

topspin

User Manual

Manual for TopSpin 2.1
Version 2.1.0



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Chapter 1

Getting Started

1.1 Document Conventions

Font Conventions

abs - commands to be entered on the command line are in courier bold italic

ProcPars - menus, buttons, icons to be clicked are in times bold italic

`fid` - filenames are in courier

name - any name which is not a filename is in times italic

File/directory Conventions

<tshome> - the TOPSPIN installation (home) directory

User Action Conventions

☞ a single user action

1. the first action of a sequence
2. the second action of a sequence
3. etc.
   a) the first action of a sub-sequence

b) the second action of a sub-sequence

c) etc.

1.2 TOPSPIN Overview

Functionality

TOPSPIN is an integrated software package for:

- Displaying NMR spectra
- Printing and plotting spectra
- Exporting displays and plots in various graphics and metafile formats
- Importing NMR data from files of various formats
- Archiving spectra in various formats such as JCAMP-DX and ZIP
- E-mailing data
- Processing 1D-6D fids and spectra: window multiplication, various transforms (Fourier, Hilbert, DOSY), phase correction, baseline correction, integration, peak picking, linear prediction, smoothing, adding spectra etc.
- Displaying multiple superimposed spectra (1D and 2D).
- Simulating 1D and multi-dimensional fids, given a pulse program and a spin system (“virtual spectrometer nmr-sim”)
- Calculating T1/T2 relaxation times
- Fitting peaks with Lorentzian and Gaussian line shape models, deconvolve overlapping peaks
- Multiplet analysis
- Automatic 1D, 2D and 3D peak picking
- Automatic 1D, 2D and 3D integration
- Line shape analysis of solids spectra
- Data acquisition with Bruker Avance type spectrometers
- Supporting automated and walk-up spectrometers (ICON-NMR)
- Remote spectrometer control including web-enabled ICON-NMR
- Adding user defined functionalities to TOPSPIN (AU programs, Macros and Python programs)

Available Documentation

In TOPSPIN 2.0 and newer the ***Help*** → ***Manuals*** submenu, contains list of available manuals for the following items:

General

Beginners Guides

Acquisition - Users Guides

Acquisition - Application Manuals

Acquisition & Processing Reference

Automation and Plotting

Analysis and Simulation

Programming Manuals

Technical Manuals

Installation Guides

Good Laboratory Practice

Each document is listed with a short description of its contents.

1.3 TOPSPIN license

TOPSPIN requires a license for startup. A license can be ordered online from:

`www.bruker-biospin.de/NMR/nmrsoftw/licenses/index.html`

If your PC controls a spectrometer, TOPSPIN will start up without a license. Furthermore, you can use TOPSPIN for developer purposes with restricted functionality. In this case you have to start it from a Windows Command prompt or Linux shell as follows;

```
topspin -developer
```

1.4 Startup TOPSPIN

Under Windows

☞ Click the TOPSPIN icon on the desktop

or

☞ Start TOPSPIN from a Command Prompt as follows:

1. Click **Start** → **Run**, enter ***cmd*** and click **OK**
2. In the Command Prompt:
   a) Enter **`cd <tshome>`**
   b) Enter **`topspin`**

   where <tshome> is the directory where TOPSPIN is installed.

Under Linux

1. Open a Linux Shell or Terminal Window
2. In the Shell/Terminal:
   a) Enter **`cd <tshome>`**
   b) Enter **`./topspin`**

   where <tshome> is the directory where TOPSPIN is installed.

Startup TOPSPIN specifying dataset

Topspin can be started with a dataset option:

1. Open a Windows Command Prompt or Linux Shell
2. Enter **topspin -j TOP_DATA:<dataset path>**

The specified dataset is automatically displayed after startup.

Examples:

topspin -j TOP_DATA:c:\bio\data\guest\nmr\exam1d_1H\1\pdata\1

topspin -j TOP_DATA:c:\bio\data\guest\nmr\exam1d_1H\1\pdata\1\1r

topspin -j TOP_DATA:c:\jcamp.dx

topspin -j TOP_DATA:c:\data-archive.zip

1.5 Configuration

After the installation of TOPSPIN, it must be configured once. TOPSPIN may be used in two different ways:

on a computer which controls a spectrometer

The command ***cf*** must be executed once, to configure the spectrometer hardware. Just type this command and follow the instructions on the screen. At the end of the dialog, further configuration commands, like ***expinstall***, are offered and can be started from there.

on a computer which is used as datastation

The only configuration command to be executed is ***expinstall***. This allows you to install pulse programs, AU programs, lists etc. Just type this command and follow the instructions on the screen, selecting ***Installation for Datastation (default)***.

Note that the commands ***cf*** and ***expinstall*** can be started from the command line or from the ***Options*** or ***Spectrometer*** menu. However, the latter menu is only available after ***cf*** has been performed once, choosing ***Installation for spectrometer***.

After the configuration has finished, TOPSPIN is ready to be used. The configuration only needs to be repeated when you have installed a new version of TOPSPIN or if your spectrometer hardware has changed.

More details on configuration can be found in chapter 16.2 and the descriptions of ***cf*** and ***expinstall*** in the Acquisition Reference Manual.

1.6 How to Display Spectra

In this chapter, opening data in standard Bruker format is described. Opening other data formats is described in chapter 4.

Please note that a standard Bruker dataset is a directory tree rather than a single file:

<*dir*>\data\<*user*>\nmr\<dataset *name*>\<*expno*>\pdata\<*procno*>

e.g.

c:\bruker\topspin\data\guest\nmr\exam1d_13C\1\pdata\1

How to Open Data from the Menu

Open the ***File*** menu and click ***Open...*** A dialog box appears. Select the first option, the Browser type ***File Chooser*** and click ***OK***. A file browser appears. Navigate to your data directory and expand it to the level of *names*, *expnos*, or *procnos* (double-click a directory to expand it). Select the desired item and click ***Display***.

The selected dataset replaces the contents of the currently selected (active) window. If no data window was displayed, a new one will be created. Alternatively, you can first create a new window by clicking ***Window*** → ***New Window*** [**`Alt`**+**`w n`**) and then open a dataset from the file browser in that window.

The file browser can also be opened by entering **`reb`** on the command line.

How to Open Data from the Browser

TOPSPIN has data browser which, by default, displays the top level data directory (<*dir*>) with Bruker example data. You can add your own data directories, local or remote, as follows:

1. Move the cursor into the browser area
2. Right-click and choose ***Add New Data Dir...*** in the popup menu
3. Enter the desired data directory (<*dir*>) and click ***OK***

Your data directory will now appear in the browser

In order to display data from the Browser, proceed as follows:

1. Expand your top level directory (<*dir*>) in the browser to the level of the data *name*, *expno* or *procno*
2. Select the desired item and drag it into the data area

How to Define Alias Names for Data

1. Open the dataset for which you want to define an alias name
2. Click the ***Alias*** tab at the top of the data browser.
3. Right-click in the browser and choose

   Define alias for data in selected window

Alternatively, you can enter the command **`dalias`** on the command line.

How to Open Data in Archive Data Directories

Topspin 2.0 and newer allows opening datasets that are stored in the following directory structures:

<mydata>/<name>/<expno>/pdata/<procno>

You can do that with the TOPSPIN command ***reb*** or from the Operating System File Browser with **Copy & Paste** or **Drag & Drop**. Actually, the data are copied to the data directory:

<tshome>/data/<user>/nmr/<name>/<expno>/pdata/<procno>

where <tshome> is the TOPSPIN installation directory and <user> is the current (internal) TOPSPIN user.

How to Open Data in Other Ways

TOPSPIN provides various other ways of displaying data. You can, for example, use command line commands like ***re***, ***rew***, ***rep*** and ***dir***. Details on these features can be found in chapter 4.3 and in the Processing Reference Manual.

1.7 How to Expand a Spectral Region

To expand a certain spectral region:

☞ Click-hold the left mouse button on one side of the region, drag the cursor to the other side and release the mouse.

If you want to cancel the expansion while dragging the mouse, just move the mouse out of the data area and release it.

An alternative way of expanding a region is clicking the  button repeatedly and then shifting the spectrum to the proper position.

1.8 How to Display Peaks, Integrals, ... together with the Spectrum

When a spectrum is displayed, you can superimpose its title, parameters, integrals, and peaks as follows:

1. Move the cursor into the data window that contains the spectrum

2. Right-click and choose ***Display Properties...*** in the popup menu
3. Check the desired items and click ***OK***

Please note that the selected items are only shown if they are available. For example, peaks and integrals are only shown if peak picking and integration have been performed, respectively (see also chapter 11). The number of displayed digits for the integral and peak labels can be set in the User Preferences (click ***Options*** → ***Preferences*** → ***Spectrum***).

1.9 How to Display Projections/1D Spectra with 2D Spectra

To display projections or 1D spectra in tandem with a 2D spectrum:

1. Open a 2D spectrum
2. If no projections are shown, click the  button in the upper toolbar or enter ***.pr*** on the command line.
3. Move the cursor into the F1 or F2 projection area.
4. Right-click and choose one of the options. With ***External Projection...*** an existing 1D spectrum can be read. This can be a regular 1D spectrum or a 2D projection that was stored as a 1D spectrum. With ***Internal Projection*** the positive projection can be calculated and displayed.

Alternate way to calculate projections is the following:

☞ Click ***Processing*** → ***Display Projections***...[***projd***]

or

☞ Right-click on a 1D dataset in the browser and choose:

Display As 2D Projection

1.10 How to Superimpose Spectra in Multiple Display

TOPSPIN allows you to compare multiple spectra in Multiple Display mode. To enter this mode, click the  button in the upper toolbar or enter ***.md*** on the command line. When you open a dataset now, for example drag one from the browser, it will be superimposed on the current spectrum rather than replacing it. Several multiple display functions are available now in the data window toolbar. Most importantly, you can *scale* and *shift* each spectrum individually. This allows exact

alignment of corresponding peaks of different spectra.

Multiple display mode is supported for 1D and 2D spectra. In 2D, you can superimpose an arbitrary number of 1D or 2D spectra.

1.11 How to Print or Export the Contents of a Data Window

How to Print Data

A TOPSPIN data window may contain various objects like an fid, a spectrum, expansions of a spectrum, superimposed spectra, spectrum components such as parameters, peaks, integrals, cross sections etc. Whatever the content of the data window is, it can be printed as follows: type ***Ctrl*+*p*** or click ***File*** → ***Print***..., select ***Print active window*** in the appearing dialog box and click ***OK***.

The other options in this dialog box enable you to use or create plot layouts. Details on this can be found in the Plot Editor manual to be found under ***Help*** → ***Manuals*** → [**Automation and Plotting**] ***TopSPin Plotting***.

The colors of the printed data can be chosen in the User Preferences dialog box. Just enter the command ***set*** or click ***Options*** → ***Preferences***... and click ***Printer*** in the left part of the dialog box.

How to Copy a Data Window to Clipboard

Under MS Windows, you can easily copy the data window contents to other applications. To do that, type ***copy*** or click ***Edit*** → ***Copy***. This will copy the data window contents to the clipboard. After that you can paste the clipboard contents to any Windows application.

How to Store (Export) a Data Window as Graphics File

The clipboard and metafile formats are resizable vector formats. In addition to this, TOPSPIN allows you to save the contents of a data window in a graphics file of selectable type, e.g. `.png`, `.jpg`, `.jpeg`, `.bmp`, `.emf` and `.wmf`. To do that, click ***File*** → ***Export***.... The resolution of such a *screen dump* equals the resolution of your screen.Note that when you import a graphics file into another program, resize, it you loose information. Therefore we recommend to resample rather than resize graphics.

1.12 How to Process Data

Since this manual is not a general NMR text book, we assume here that you are familiar with terms like window multiplication, Fourier Transform, phase correction, etc.

Any Fid or a spectrum displayed in a TOPSPIN window can be processed by:

- typing a command on the command line, e.g. ***ft***
- invoking a command from the ***Processing*** or ***Analysis*** menu, e.g. ***Processing → Fourier Transform...***
- entering an interactive mode by clicking a tool button, e.g. 
- entering a user defined command (usually an AU or a Python program, see ***Help → Manuals*** [**Programming Manuals**].

Processing and analysis commands require certain parameters to be set correctly. Most commands in the ***Processing*** or ***Analysis*** menu, like ***wm*** and ***ftf*** open a dialog box showing the available options and required parameters for that command. Other commands such as ***em***, ***ft***, ... start processing immediately. Before you use them, you must set their parameters from the parameter editor. To do that, enter ***edp*** or click the ***ProcPars*** Tab of the data window.

If you are a new or occasional user we recommend you to process your data with the TOPSPIN Processing Guide. This will guide you through the typical sequence of processing steps. To start the Processing Guide, click ***Processing → Processing Guide***. In ***Automatic mode***, the Processing Guide will simply execute each processing command when you click the corresponding button. This requires the processing parameters to be set correctly. In interactive mode (***Automatic mode*** unchecked), the Processing Guide will, at each step, open a dialog box offering you the available options and required parameters. For example, the phase correction button offers various automatic algorithms as well as an option to enter interactive phasing mode.

A simple way to process 1D data is the following:

1. Click ***Processing → Process / Plot Current data***
2. In the appearing dialog (see Fig. 1.1):
   a) Enable the desired processing/plotting steps
   b) Set the parameter LB for Exponential multiplication

c) Select the desired LAYOUT for plotting.

d) Click ***OK***

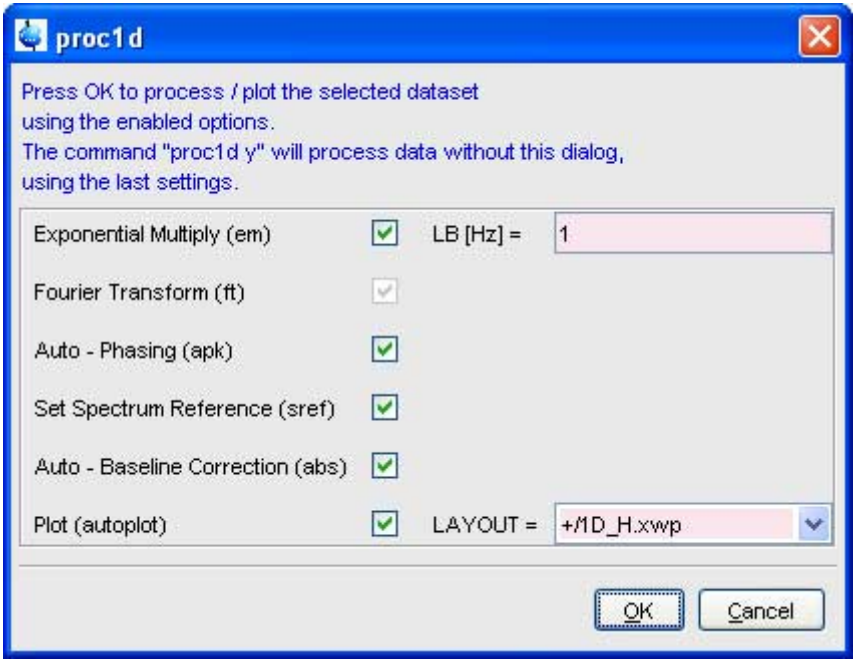


Figure 1.1

1.13 How to Archive Data

TOPSPIN 2.1 provides the following methods for data archiving:

- Automatic archiving of raw data after the acquisition as defined in the User preferences (click ***Options*** → ***Preferences*** → ***Acquisition*** → ***Configure ...)***
- Copying a dataset to a desired destination directory which could for instance be located on a server. Type ***wrpa***, click ***File*** → ***Save...*** or type ***Ctrl***+***s***.
- Saving a dataset in a ZIP file. A standard Bruker dataset is a directory tree which contains several files. “Zipping” a dataset stores the entire data directory tree into a single file with the extension `.bnmr.zip`. To zip a dataset, type ***tozip***, click ***File*** → ***Save...*** or type ***Ctrl***+***s***. To unpack and display a

zipped dataset, enter ***fromzip***. Note that `.bnmr.zip` files are fully compatible with the well known PC zip format and can be unpacked with any common unzip utility. “Zipping” can be applied to 1D, 2D, 3D and 4D data.

- Saving a dataset in JCAMP-DX format. This format is a IUPAC standard, and is available for 1D and 2D datasets. Data and parameters are stored in readable text (ASCII) format. To store data in JCAMP, type ***tojdx***, click ***File*** → ***Save...*** or type ***Ctrl***+***s***. To convert and display a JCAMP-DX file, type ***fromjdx***.
- E-mailing data to a desired destination. Type ***smail*** or click ***File*** → ***Send To...***. The mailing format is either zip or JCAMP-DX, both of which allow for data compression in order to keep the transferred data size as small as possible.

1.14 How to Import NMR Data Stored in Special Formats

TOPSPIN allows you to convert various data formats to standard Bruker format for display and processing. Click ***File*** → ***Open...*** and select ***Open NMR data stored in special formats***. Then follow the instruction on the screen.

1.15 How to Fit Peaks and Deconvolve Overlapping Peaks

Peaks of a 1D and 2D NMR spectrum can be approximated by a Lorentzian, Gaussian, or a mixture of these line shapes. Overlapping peaks may be deconvolved into a sum of such line shapes.

TOPSPIN shows the deconvolution result, i.e. peak positions, line widths and integrals on the screen and stores it in the file `dconpeaks.txt`. Furthermore, it switches to multiple display mode to show the original spectrum and the sum of the computed line shapes, superimposed.

To start deconvolution, expand the spectrum on the display to show the peak or peak group of interest. Then type ***dcon*** or click ***Analysis*** → ***Deconvolution...***.

1.16 How to Compute Fids by Simulating Experiments

TOPSPIN includes a “virtual spectrometer” that computes fids of any dimension. A “real” spectrometer excites a sample with high frequency pulses defined by a pulse

program and measures the resulting fid. The virtual spectrometer performs this task mathematically by solving the quantum mechanical Liouville equation. The "sample" must be entered in form of a spin system description. For the computation, the same pulse program and acquisition parameters are taken as for the real experiment. The result is a time domain signal which can be processed with TOPSPIN in the same way a measured fid is processed. Techniques such a selective excitation, gradient enhanced spectroscopy, and the handling of mixtures are supported.

To start the virtual spectrometer:

☞ Enter ***nmrsim*** on the command line or click ***Analysis*** → ***Simulate Fid...***.

1.17 How to Add Your Own Functionalities

The TOPSPIN functionality can be extended with various user defined commands, programs etc.

How to Create Macros

Writing a macro is the simplest way to create a user defined command. Just enter the command ***edmac***, select a file, and enter a sequence of regular TOPSPIN commands and/or Python commands. Save the file under a name of your preference. You have created a new TOPSPIN command. Just enter its name on the command line to execute it.

The command ***xmac*** shows a list of all available macros and allows you to execute one.

How to Create AU (automation) Programs

Writing an AU program is another way of creating a new TOPSPIN command. AU programs are more complex and more powerful then macros. They are C-language programs, which may contain C-statements, regular TOPSPIN commands, and various predefined AU macros and functions. AU programs can perform various tasks such as dataset handling, parameter handling, acquisition, processing, analysis, and printing. Note that AU programs do not support graphics related tasks.

TOPSPIN is delivered with a large set of Bruker AU programs for data processing and acquisition. Just enter ***edau*** to see them listed in a dialog box. The easiest

way to create a new AU program is to select a Bruker AU program, save it under a new name and modify it to your needs. The chosen name is now available as a new TOPSPIN command. Alternatively, you can open a new file from the AU dialog box and write your AU program from scratch.

For details on Bruker AU programs and writing your own AU programs, click ***Help*** → ***Manuals*** → [**Programming Manuals**] ***AU Programming***.

How to Create Python Programs

Writing a Python program is yet another way of creating a new TOPSPIN command. Python is a new generation scripting and object oriented programming language. Python programs are even more powerful than AU programs. They are easy to use and allow you to execute TOPSPIN commands, handle NMR data and parameters, generate graphics, and interact with the TOPSPIN user interface via dialogs, windows etc. To create a Python program, enter the command ***edpy***, select a file and insert your Python statements. Graphics and interface features programmed in Python look and work the same as regular TOPSPIN features.

For details on Python programming, click ***Help*** → ***Manuals*** → [**Programming Manuals**] ***Python Programming***. The examples mentioned there, like *pycmd1*, are delivered with TOPSPIN. Just enter their names on the command line to execute them.

The Python dialog window is also available from the TOPSPIN menu:

☞ Click ***File*** → ***Open...***and select ***Open other file*** → ***Python program***.

1.18 How to Automate Data Acquisition

TOPSPIN provides special user interfaces for automation, walk-up, bio-molecular experiments, etc. To open these interfaces:

☞ Type ***iconnmr*** or click ***Spectrometer*** → ***ICONNMR***.

Chapter 2

The TOPSPIN Interface

2.1 The Topspin Window

The TOPSPIN window consists of a data area, a data browser, toolbars and a menu-bar. Note that the browser can be inactive [hit ***Ctrl***+***d***] or displayed as a separate window.

Fig. 2.1 shows the Topspin window with two data windows in the data area and the browser as an integral part.

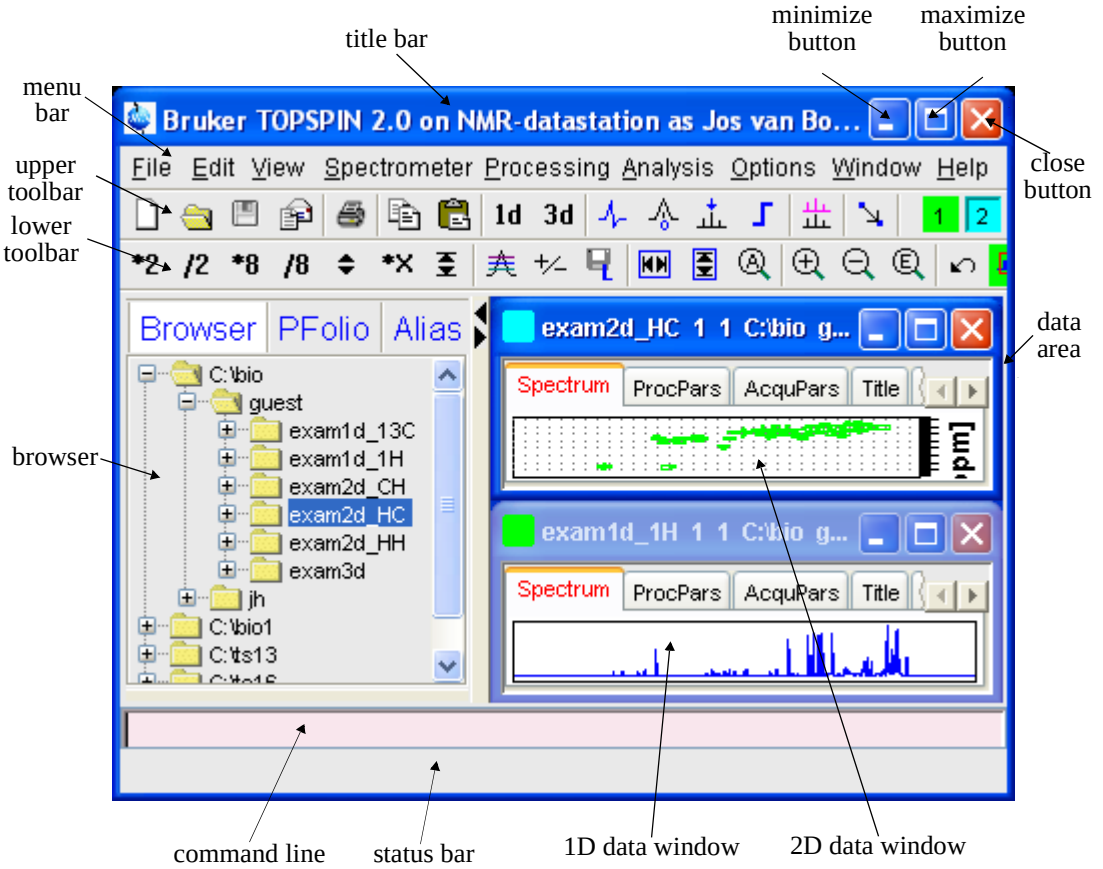


Figure 2.1

Note that the menus and toolbars depend on the data dimensionality. The descriptions below hold for 1D data. For 2D and 3D data, the menus and toolbars are similar and will be discussed in the chapters 9, 10 and 12, respectively.

How to Use Multiple Data Windows

TOPSPIN allows you to use multiple data windows. Data windows can be opened from the browser or from the ***Window*** menu. They can contain the same of different datasets. Data windows can be arranged from the ***Window*** menu. One of them is the active (current) data window. The active data window:

- is the only data window receiving commands from the command line

- can be selected by clicking inside the window or hitting F6 repeatedly.
- has a highlighted title bar
- has the mouse focus

A cursor line (1D) or crosshair (2D) is displayed in all data windows at the same position. Moving the mouse affects the cursor in all data windows.

How to Use the Menu bar

The menu bar contains the following menus:

- ***File*** : performing data/file handling tasks
- ***Edit*** : copy & paste data and finding data
- ***View*** : display properties, browser on/off, notebook, command history
- ***Spectrometer*** : data acquisition and acquisition related tasks
- ***Processing*** : data processing
- ***Analysis*** : data analysis
- ***Options*** : setting various options, preferences and configurations
- ***Window*** : data window handling/arrangement
- ***Help*** : access various information, indices, manuals etc.

Experienced users will usually work with keyboard commands rather than menu commands. Note that the main keyboard commands are displayed in square brackets [] behind the corresponding menu entries. Furthermore, right-clicking any menu entry will show the corresponding command.

How to Use the Upper Toolbar (1D data)

The upper toolbar contains buttons for data handling, switching to interactive modes, display settings, and starting acquisition.

Buttons for data handling:



The functions of the individual buttons are:

 Create a new dataset[***Ctrl***+***n***, ***new***]

 Open a dataset [***Ctrl***+***o***, ***open***]

Save the current dataset [***Ctrl***+***s***, ***sav***]

Email the current dataset[***smail***]

Print the current dataset [***Ctrl***+***p***, ***print***]

Copy the data path of the active data window to the clipboard [***copy***]

Paste the data path on the clipboard to the active data window [***paste***]

Switch to the last 2D dataset [***.2d***]

Switch to the last 3D dataset [***.3d***]

For more information on dataset handling, please refer to chapter 4.3.

Buttons for interactive functions



The functions of the individual buttons are:

Enter phase correction mode

Enter calibration mode

Enter baseline correction mode

Enter peak picking mode

Enter integration mode

Enter multiple display mode

Enter distance measurement mode

For more information on interactive functions, refer to chapter 11 and 12.

Buttons for display options



The functions of the individual buttons are:


Toggle between Hz and ppm axis units


Switch the y-axis display between abs/rel/off


Switch the overview spectrum on/off


Toggle grid between fixed/axis/off

How to Use the Lower Toolbar (1D data)

The lower toolbar contains buttons for display functions.

Buttons for vertical scaling (intensity)




Increase the intensity by a factor of 2 [***2***]


Decrease the intensity by a factor of 2 [***/2***]


Increase the intensity by a factor of 8 [***8***]


Decrease the intensity by a factor of 8 [***/8***]


Change the intensity smoothly


Reset the intensity (baseline positions remains unchanged) [***.vr***]

Note that vertical scaling can also be changed with the mouse wheel.

Buttons for horizontal scaling (zooming):




Reset zooming (horizontal scaling) to full spectrum [***.hr***]


Display the entire spectrum (baseline position and intensity scaling are adjusted if necessary) [***.all***]


Zoom in to the center (spectrum) or left edge (FID) of the displayed re-

gion, increasing the horizontal scaling. [***.zi***]

Zoom in/out smoothly

Zoom out from the center (spectrum) or left edge (FID) of the displayed region, decreasing horizontal scaling) [***.zo***]

Exact zoom via dialog box[***.zx***]

Toggle interactive zoom mode. When switched off, interactive zooming only selects a horizontal region; baseline position and intensity scaling remain the same. When switched on, interactive zooming draws a box selecting the corresponding area.

Undo last zoom [***.zl***]

Retain horizontal and vertical scaling when modifying dataset or changing to different dataset. Global button for all data windows [***.keep***]

Buttons for horizontal shifting



Shift to the left, half of the displayed region [***.sl***]

Smoothly shift to the left or to the right

Shift to the right, half of the displayed region [***.sr***]

Shift to the extreme left edge of the spectrum [***.sl0***]

Shift to the extreme right edge of the spectrum [***.sr0***]

Buttons for vertical shifting



Shift the spectrum baseline to the middle of the data field [***.su***]

Smoothly shift the spectrum baseline up or down.

Shift the spectrum baseline to the bottom of the data field [***.sd***]

For more information on display options, please refer to chapter 8.5 (1D data) and 9.5 (2D data).

2.2 Command Line Usage

How to Put the Focus in the Command Line

In order to enter a command on the command line, the focus must be there. Note that, for example, selecting a dataset from the browser, puts the focus in the browser. To put the focus on the command line:

☞ Hit the ***Esc*** key

or

☞ Click inside the command line

How to Retrieve Previously Entered Commands

All commands that have been entered on the command line since TOPSPIN was started are stored and can be retrieved. To do that:

☞ Hit the ↑ (***Up-Arrow***) key on the keyboard

By hitting this key repeatedly, you can go back as far as you want in retrieving previously entered commands. After that you can go forward to more recently entered commands as follows:

☞ Hit the ↓ (***Down-Arrow***) key on the keyboard

How to Change Previously Entered Commands

1. Hit the ← (***Left-Arrow***) or → (***Right-Arrow***) key to move the cursor
2. Add characters or hit the ***Backspace*** key to remove characters
3. Mark characters and use ***Backspace*** or ***Delete*** to delete them, ***Ctrl***+***c*** to copy them, or ***Ctrl***+***v*** to paste them.

In combination with the arrow-up/down keys, you can edit previously entered commands.

How to Enter a Series of Commands

If you want to execute a series of commands on a dataset, you can enter the commands on the command line separated by semicolons, e.g.:

```
em;ft;apk
```

If you intend to use the series regularly, you can store it in a macro as follows:

☞ right-click in the command line and choose ***Save as macro***.

2.3 Command Line History

TOPSPIN allows you to easily view and reuse all commands, which were previously entered on the command line. To open a command history control window; click ***View*** → ***`Command Line History`***, or right-click in the command line and choose ***`Command Line History`***, or enter the command ***`cmdhist`*** (see Fig. 2.2).

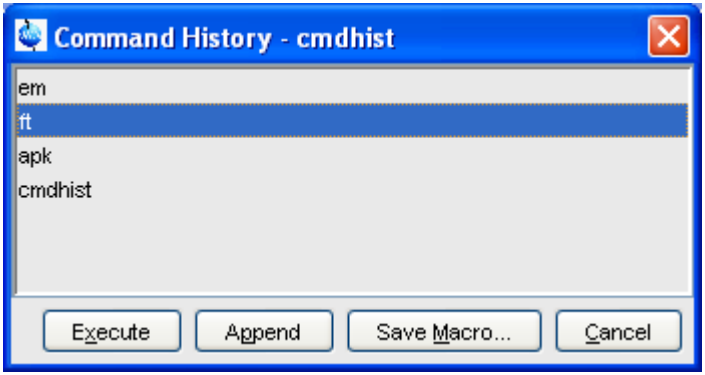


Figure 2.2

It shows all commands that have been entered on the command line since TOPSPIN was started. You can select one or more commands and apply one of the following functions:

Execute

Execute the selected command(s).

Append

Append the (first) selected command to the command line. The appended

command can be edited and executed. Useful for commands with many arguments such as ***re***.

Save as..

The selected command(s) are stored as a macro. You will be prompted for the macro name. To edit this macro, enter ***edmac <macro-name>***. To execute it, just enter its name on the command line.

2.4 Starting TOPSPIN commands from a Command Prompt

TOPSPIN commands can be executed outside of the TOPSPIN interface, from a Windows Command Prompt or Linux Shell.

Under Windows

1. Open a Windows Command Prompt
2. Enter a TOPSPIN command in the following format:

   <tshome>\prog\bin\sendgui <topspincommand>

   where <tshome> is the TOPSPIN installation directory.

Examples:

C:\ts2.1\prog\bin\sendgui ft

executes a 1D Fourier transform.

C:\ts2.1\prog\bin\sendgui re exam1d_1H 1 1 C:/bio joe

reads the dataset C:/bio/joe/nmr/exam1d_13C/1/pdata/1.

Under Linux

1. Open a Linux Shell
2. Enter a TOPSPIN command in the following format:

   <tshome>\prog\bin\scripts\sendgui <topspincommand>

   where <tshome> is the TOPSPIN installation directory.

   or

   sendgui <topspincommand>

if the TOPSPIN home directory is in the users search path.

Examples:

```
C:\ts2.1\prog\bin\scripts\sendgui ft
```

executes a 1D Fourier transform.

```
sendgui re exam1d_1H 1 1 C:/bio joe
```

reads the dataset C:/bio/joe/nmr/exam1d_13C/1/pdata/1.

Note that commands are executed on the currently active TOPSPINdata window.

2.5 Function Keys and Control Keys

For several TOPSPIN commands or tasks, you can use a control-key or function-key short cut.

Focus anywhere in TOPSPIN

Esc	Put the focus in the command line
Shift+Esc	Display menu bar and toolbars (if hidden)
F2	Put the focus in the browser
F1	Search for string in command help or NMR Guide [***help***]
F6	Select the next window in the data area
Alt+***F4***	Terminate TOPSPIN [***exit***]
Ctrl+***d***	Switch the browser on/off
Ctrl+***o***	Open data [***open***]
Ctrl+***f***	Find data [***find***]
Ctrl+***n***	New data [***new***]
Ctrl+***p***	Print current data [***print***]
Ctrl+***s***	Save current data [***sav***]
Ctrl+***w***	Close active window [***close***]
Ctrl+***c***	Copy a text that you selected/highlighted in an error box, dialog box, pulse program, title etc., to the clipboard
Ctrl+***v***	Paste text from the clipboard into any editable field.

Focus in the Command Line

Ctrl*+*Backspace	Kill current input
Ctrl*+*Delete	Kill current input
UpArrow	Select previous command (if available).
DownArrow	Select next command (if available).

Focus in the Browser

UpArrow	Select previous dataset
DownArrow	Select next dataset
Enter	dir/user/name/expno selected: expand node or collapse node, depending on the current state
Enter	procno selected: display this dataset
Ctrl+Enter	name/expno selected: display this dataset
Enter	multiple procnos selected: show in multiple display
Delete	one or more name/expno/procno nodes selected: delete these datasets

Focus anywhere in TOPSPIN

Scaling Data	
Alt+PageUp	Scale up the data by a factor of 2 [***2**]
Alt+PageDown	Scale down the data by a factor 2 [**/2**]
Ctrl+Alt+PageUp	Scale up by a factor of 2, in all data windows
Ctrl+Alt+PageDown	Scale down by a factor of 2, in all data windows
Alt+Enter	Perform a vertical reset
Ctrl+Alt+Enter	Perform a vertical reset in all data windows
Zooming data	
Alt+Plus	Zoom in [**.zi**]
Alt+Minus	Zoom out [**.zo**]
Ctrl+Alt+Plus	Zoom in, in all data windows
Ctrl+Alt+Minus	Zoom out, in all data windows
Shifting Data	
Alt+UpArrow	Shift spectrum up [**.su**]
Alt+DownArrow	Shift spectrum down [**.sd**]
Alt+LeftArrow	Shift spectrum to the left [**.sl**]
Alt+RightArrow	Shift spectrum to the right [**.sr**]
Ctrl+Alt+UpArrow	Shift spectrum up, in all data windows
Ctrl+Alt+DownArrow	Shift spectrum down, in all data windows
Ctrl+Alt+LeftArrow	Shift spectrum to the left, in all data windows
Ctrl+Alt+RightArrow	Shift spectrum to the right, in all data windows

Focus in a Table (e.g. peaks, integrals, nuclei, solvents)

delete	Delete the selected entries
home	Select the first entry
end	Select the last entry
Shift+Home	Select the current and first entry and all in between
Shift+End	Select the current and last entry and all in between
DownArrow	Select next entry
UpArrow	Select previous entry
Ctrl+a	Select all entries
Ctrl+c	Copy the selected entries to the clipboard
Ctrl+z	Undo last action
Ctrl+y	Redo last undo action

Focus in a Plot Editor

F1	Open the Plot Editor Manual
F5	Refresh
Ctrl+F6	Display next layout
ctrl*+*Shift*+*F6	Display previous layout
Ctrl*+*tab	Display next layout
delete	Delete the selected objects
Ctrl*+*a	Select all objects
Ctrl*+*i	Open TOPSPIN Interface
Ctrl*+*c	Copy the selected object from the Clipboard
Ctrl*+*l	Lower the selected object
Ctrl*+*s	Save the current layout
Ctrl*+*m	Unselect all objects
Ctrl*+*n	Open a new layout
Ctrl*+*o	Open an existing layout
Ctrl*+*p	Print the current layout
Ctrl*+*q	Close the Plot Editor window (Linux only)
Ctrl*+*r	Raise the selected object
Ctrl*+*t	Reset X and Y scaling of all marked objects
Ctrl*+*v	Paste the object from the Clipboard
Ctrl*+*w	Open the attributes dialog window.
Ctrl*+*x	Cut the selected object and place it on the Clipboard
Ctrl*+*z	Undo the last action

Note that the function of function keys can be changed as described in chapter 2.7.

2.6 Help in Topspin

TOPSPIN offers help in various ways like online manuals, command help and tooltips.

How to get a Panorama Tour

For a quick overview over TOPSPIN Interface, Acquisition, Processing, Analysis and Documentation:

☞ Click ***Help*** → ***Panorama Tour***

How to Open Online Help documents

The online help manuals can be opened from the ***Help*** → ***Manuals*** submenu. For example, to open the manual that you are reading now:

☞ Click ***Help*** → ***Manuals*** → [**General**] ***User Manual***

To open the Avance Beginners Guide:

☞ Click ***Help*** → ***Manuals*** → [**Beginners Guides**] <***language***>

To open the Processing Reference guide:

☞ Click ***Help*** → ***Manuals*** → [**Acquisition & Processing References**] ***Proc. Commands and Parameters***

Note that most manuals are stored in the directory:

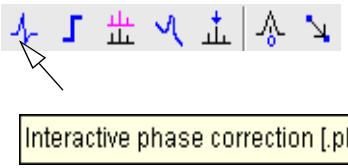
<tshome>/prog/docu/english/xwinproc/pdf

The most recent versions can be downloaded from:

`www.bruker-biospin.de`

How to Get Tooltips

If you hold the cursor over a button of the toolbar, a tooltip will pop up. This is a short explanation of the buttons function. For example, if you hold the cursor over the interactive phase correction button, you will see the following:



The corresponding command line command, in this case ***.ph***, is indicated between square brackets.

Note that the tooltip also appears in the status bar at the bottom of the TOPSPIN window.

How to Get Help on Individual Commands

To get help on an individual command, for example ***ft***:

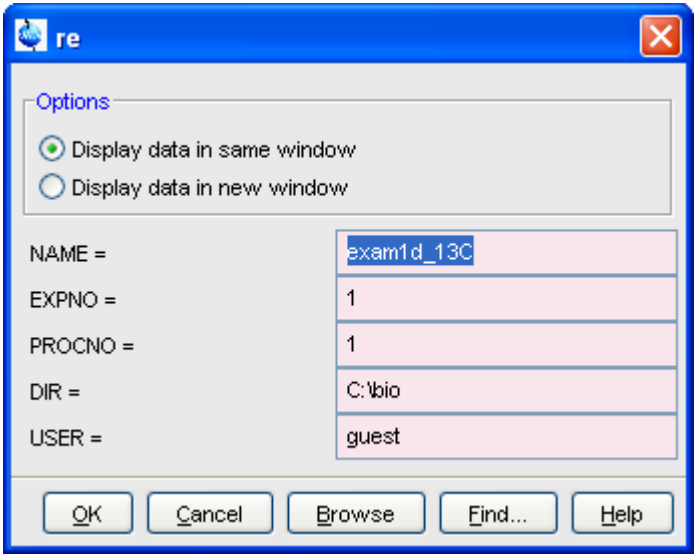
☞ Enter ***ft?***

or

☞ Enter ***help ft***

In both cases, the HTML page with a description of the command will be opened.

Note that some commands open a dialog box with a ***Help*** button. Clicking this button will show the same description as using the ***help*** command. For example, entering ***re*** and clicking the ***Help*** button in the appearing dialog box



opens the same HTML file as entering ***help re*** or ***re?***.

How to Use the Command Index

To open the TOPSPIN command index:

☞ Enter ***cmdindex***

or

☞ Click ***Help*** → ***Command Index***

From there you can search for and click any command and jump to the corresponding help page.

2.7 User Defined Functions Keys

The default assignment of functions keys is described in chapter 2.5 and in the document:

☞ Click ***Help*** → ***Manuals*** → [**General**] ***Control & Function Keys***

You may assign your own commands to functions keys. Here is an example of how to do that:

1. Open the file `cmdtab_user.prop`, located in the subdirectory `userdefined` of the user properties directory (to locate this directory, enter ***`hist`*** and look for the entry "User properties directory="). The file `cmdtab_user.prop` is initially empty and can be filled with your own command definitions.
2. Insert e.g. the following lines into the file:

```
_f3=$em
_f3ctrl=$ft
_f3alt=$pk
_f5=$halt
_f5ctrl=$reb
_f5alt=$popt
```

3. Restart TOPSPIN

Now, when you hit the ***`F3`*** key, the command ***`em`*** will be executed. In the same way, ***`Ctrl`***+***`F3`***, ***`Alt`***+***`F3`***, ***`F5`***, ***`Ctrl`***+***`F5`*** and ***`Alt`***+***`F5`*** will execute the commands ***`ft`***, ***`pk`***, ***`halt`***, ***`reb`*** and ***`popt`***, respectively. You can assign any command, macro, AU program or Python program to any function keys. Only the keys ***`Alt`***+***`F4`***, ***`F6`***, ***`Ctrl`***+***`F6`***, and ***`Alt`***+***`F6`*** are currently fixed. Their function cannot be changed.

2.8 How to Open Multiple TOPSPIN Interfaces

TOPSPIN allows you to open multiple User Interfaces. This is, for example, useful to run an acquisition in one interface and process data in another. To open an addition interface, enter the command ***`newtop`*** on the command line or click ***Window*** → ***New Topspin***. To open yet another interface, enter ***`newtop`*** in the first or in the second interface. The display in each interface is completely independent from the others. As such, you can display different datasets or different aspects of the same

dataset, e.g. raw/processed, regions, scalings etc. When the dataset is (re)processed in one interface, its display is automatically updated in all TOPSPIN interfaces.

The command ***exit*** closes the current Topspin interface. Interfaces that were opened from this interface remain open. Entering ***exit*** in the last open TOPSPIN interface, finishes the entire TOPSPIN session. The position and geometry of each TOPSPIN interface is saved and restored after restart.

Chapter 3

Trouble Shooting

3.1 General Tips and Tricks

On a spectrometer, make sure the commands ***cf*** and ***expinstall*** have been executed once after installing TOPSPIN. ***cf*** must be executed again if your hardware configuration has changed. Sometimes, executing ***cf*** is useful in case of acquisition problems.

On a datastation, a default configuration is automatically done during the installation. No configuration commands are required. Only if you want to use AU programs, you must run ***expinstall*** once.

3.2 History, Log Files, Spooler Reports, Stack Trace

If you have a problem with TOPSPIN and want to contact Bruker, it is useful to have as much information as possible available. If TOPSPIN is still running, you can view log files with the commands ***hist*** and ***ptrace***. If TOPSPIN hangs, you can create a stack trace by hitting **Ctrl+** (Linux) or **Ctrl+Break** (Windows) in the TOPSPIN startup window.

3.2.1 TOPSPIN command-log

By default, the history (protocol) feature is switched on.This means all TOPSPIN commands will be protocolled and can be examined by entering ***hist*** on the command line.

If, for some reason, history is switched off, you can switch it on as follows:

1. Click ***Options*** → ***Preferences***, click ***Miscellaneous***
2. Check the entry "*Record commands in protocol file*"
3. Click ***OK***.

3.2.2 TOPSPIN spooler report

TOPSPIN reports all queued, delayed and cron jobs in the so called spooler report file. The spooler report stores all jobs since TOPSPIN installation and can become very large. Therefore it should be cleaned from time to time. To do that:

1. Enter the command ***spooler***
2. Click ***Tools*** → ***Show spooler report***
3. Mark the entries to be deleted
4. Right-click in the dialog and choose ***Delete***.
5. Close the Spooler report.

Note that the spooler report can also be opened from Spooler field (if enabled) in the Acquisition Status Bar by right-clicking the word **Spooler** and choosing ***Show spooler report***.

3.2.3 TOPSPIN command, dataserver and network log

A full protocol including not only TOPSPIN commands but also dataserver and network traffic is show by the command ***ptrace***. This opens the following dialog

window:

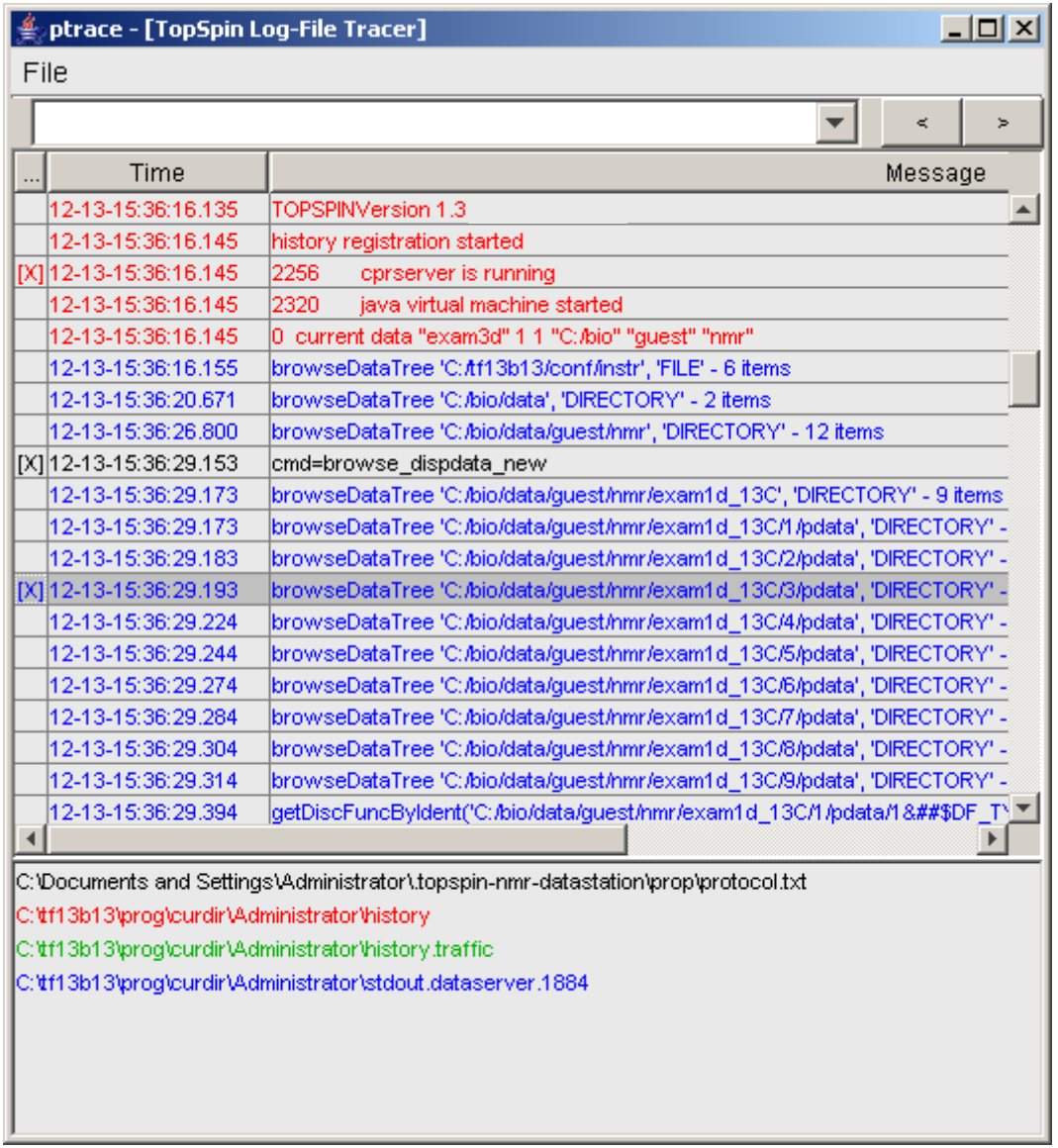

ptrace - [TopSpin Log-File Tracer]
File
...
Time
Message
12-13-15:36:16.135 TOPSPINVersion 1.3
12-13-15:36:16.145 history registration started
[X] 12-13-15:36:16.145 2256 cprserver is running
12-13-15:36:16.145 2320 java virtual machine started
12-13-15:36:16.145 0 current data "exam3d" 1 1 "C:/bio" "guest" "nmr"
12-13-15:36:16.155 browseDataTree 'C:/tf13b13/conf/instr', 'FILE' - 6 items
12-13-15:36:20.671 browseDataTree 'C:/bio/data', 'DIRECTORY' - 2 items
12-13-15:36:26.800 browseDataTree 'C:/bio/data/guest/nmr', 'DIRECTORY' - 12 items
[X] 12-13-15:36:29.153 cmd=browse_dispdata_new
12-13-15:36:29.173 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C', 'DIRECTORY' - 9 items
12-13-15:36:29.173 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/1/pdata', 'DIRECTORY' -
12-13-15:36:29.183 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/2/pdata', 'DIRECTORY' -
[X] 12-13-15:36:29.193 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/3/pdata', 'DIRECTORY' -
12-13-15:36:29.224 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/4/pdata', 'DIRECTORY' -
12-13-15:36:29.244 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/5/pdata', 'DIRECTORY' -
12-13-15:36:29.274 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/6/pdata', 'DIRECTORY' -
12-13-15:36:29.284 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/7/pdata', 'DIRECTORY' -
12-13-15:36:29.304 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/8/pdata', 'DIRECTORY' -
12-13-15:36:29.314 browseDataTree 'C:/bio/data/guest/nmr/exam1d_13C/9/pdata', 'DIRECTORY' -
12-13-15:36:29.394 getDiscFuncByIdent('C:/bio/data/guest/nmr/exam1d_13C/1/pdata/1&##$DF_T
C:\Documents and Settings\Administrator\.topspin-nmr-datastation\prop\protocol.txt
C:\tf13b13\prog\curdir\Administrator\history
C:\tf13b13\prog\curdir\Administrator\history.traffic
C:\tf13b13\prog\curdir\Administrator\stdout.dataserver.1884

Figure 3.1

Here TOPSPIN log messages from various log files are displayed time sorted.

Messages from different log files are shown in different colours. The color assignment and location of the files is shown in the lower part of the dialog window.

ptrace supports the following functions:

Search keywords

To search the displayed log files for a certain keyword, just enter it in the text bar at the top of the window and hit Enter.

Anchor specific entries

To anchor an entry:

double-click in the first column of the entry

The entry is marked with an **X**. Now you can use the < > buttons at the upper right of the window to go to the previous or next entry, respectively.

Add log files

By default, the `procol.txt`, `history` and `dataserver` log files are shown.To include additional log files to the ***ptrace*** list:

click ***File*** → ***Add***, specify the file and click ***Open***.

Note that most log files are stored in the directory:

<tshome>/prog/curdir/<user>

Save the log messages

To save log messages in a text file;

click ***File*** → ***Save*** and specify the output text file

3.2.4 Create a Stack Trace

If TOPSPIN hangs it can be useful to sent Bruker a stack trace about a possible cause. You can create a stack trace as follows.

1. Move the cursor into the TOPSPIN startup window.
2. Under Windows: hit ***Ctrl+Break*** (***=Ctrl+Pause***)
   Under Linux: hit ***Ctrl+*** (Control backslash)
3. Copy the appearing text into a text file.

3.2.5 Store complete log

A complete set of TOPSPIN and ICON-NMR log files can be made. This contains all possible log files and is the most complete debugging information.

3.2.6 Under Windows

1. Double-click the **Utilities** icon on the desktop.
2. In the appearing window:
3. Double-click the **Miscellaneous** folder icon
4. Under Windows: double-click the **savelogs** command
   Under Linux: hit ***Ctrl+*** (Control backslash)
5. Send the file `logfiles.tar.gz` as attachment to the Bruker Service.

3.3 How to Show or Kill TOPSPIN processes

To show the currently running TOPSPIN processes, enter the command ***show*** or ***kill*** on the command line. A list of processes will appear showing the process command, dataset etc.

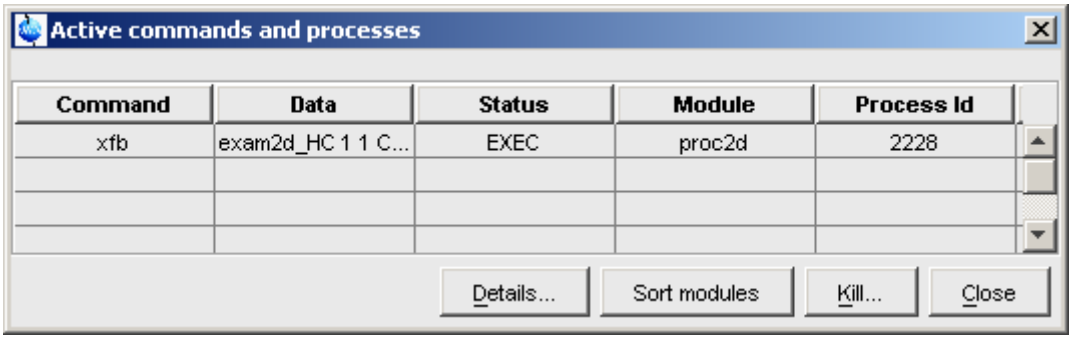


Figure 3.2

Fig. 3.2 shows a list with one process (command ***xfb***). To kill a process, select it in the list and click the button ***Kill...***

The command ***show all*** or ***kill all*** work like ***show*** and ***kill***, except that they also show TOPSPIN system processes. Note that killing such processes may kill TOPSPIN.

3.4 What to do if TOPSPIN hangs

If, for some reason, TOPSPIN hangs, please do the following.

Under Linux:

1. Open a Shell
2. Enter ***<tshome>/prog/bin/script/killtopspin***

   where <tshome> is the TOPSPIN installation directory.

Under Windows:

1. Click **Start → Programs → Bruker TOPSPIN → TOPSPIN 2.1 → Bruker Utilities 2.1**
2. In the appearing window:

   Click **killtopspin**.

Normally, this kill all TOPSPIN processes including *cpr*, *cprserver*, *dataserver* and *java*.

3.5 How to Restart User Interface during Acquisition

If Topspin hangs up during a data acquisition, you can restart the user interface without disturbing the acquisition. To do that:

1. Open the file:

   <tshome>/prog/curdir/<user>/history

   where <tshome> is the TOPSPIN home directory and <user> is the user who started TOPSPIN. Look for the term 'Java Virtual Machine' and check its PID.
2. Open the Task Manager (Windows) or System Monitor (Linux)
3. Stop the Java(w).exe process with the PID found in the history file.
4. Open a Windows Command Prompt or Linux Shell
5. Go to the TOPSPIN Installation directory
6. Enter **topspin -client**

Chapter 4

Dataset Handling

4.1 The Topspin Browser

TOPSPIN offers a data browser from which you can browse, select, and open data.

The browser dialog offers the following tabs (see Fig. 4.1):

- ***Browser*** - data browser showing the data directory hierarchy
- ***Last50*** - list of the 50 last open datasets
- ***Groups*** - list of user defined groups of datasets
- ***Alias*** - list of user defined alias name

The browser appears at the left of the TOPSPIN window and can be shown/hidden with ***Ctrl+d*** or by clicking the arrow buttons at the upper right of the browser.

The Browser tab

The browser shows data directory trees and allows you to expand/collapse their elements. Figure 4.1 shows the browser with three top level data directories and one dataset fully expanded.

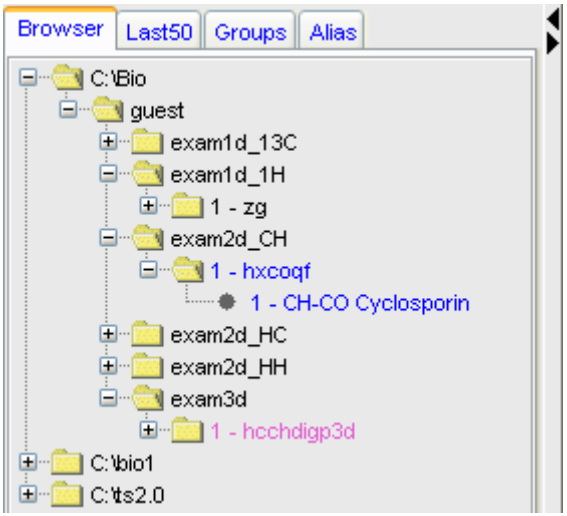


Figure 4.1

The dimensionality of the data is indicated with different colors:

- black for 1D data
- blue for 2D data
- magenta for 3D data

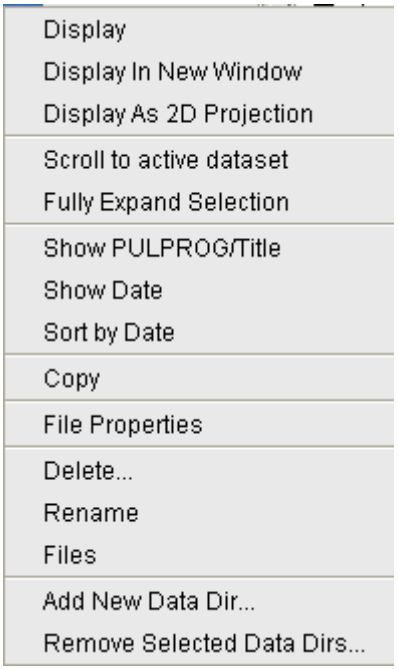
Furthermore, the browser shows:

- the pulse program with the dataset EXPNO (e.g. 1 - hxcoqf in Fig. 4.1)
- the title with the dataset PROCNO (e.g. CH-CO Cyclosporin in Fig. 4.1)

Note that the displayed pulse program is the :

- status pulse program if an acquisition has been done (raw data exist)
- setup pulse program if no acquisition has been done (raw data do not exist)

The display of title and pulse program can be switched of (see Fig. 4.2).



→ Display in current data window.
→ Display in new data window.
→ Display 1D data as projection of active 2D data.
→ Scroll to PROCNO of active data window.
→ Fully expand selected node.
→ Switch pulsprogram/title display on/off.
→ Show acq. date (expno) or last mod. date (name)
→ Sort data by last modified date
→ Copy dataset entry to clipboard
→ Show dataset properties.
→ Delete selected entry (name,expno or procno)
→ Rename dataset name, expno or procno.
→ Show files in selected entry (expno or procno)
→ Add new top level data directory.
→ Remove selected top level data directory

Figure 4.2

The Last50 tab

Clicking the ***Last50*** tab displays the list of the last 50 displayed datasets. Each dataset that you open, is automatically added to the current list. Fig. 4.3 shows a ***Last50*** list with four datasets. As in the browser, different colors are used to indicate the data dimensionality.

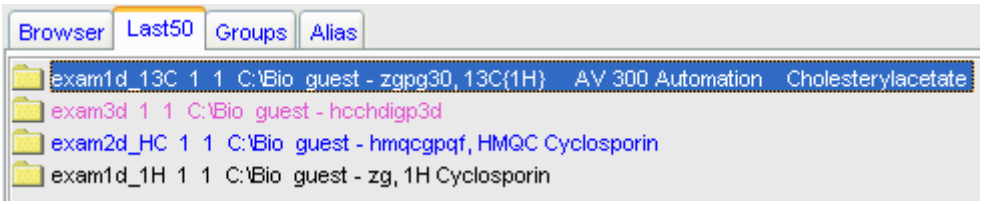
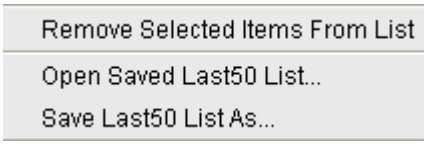

Browser
Last50
Groups
Alias
exam1d_13C 1 1 C:\Bio guest - zgpg30, 13C{1H} AV 300 Automation Cholesterylacetate
exam3d 1 1 C:\Bio guest - hcchdigp3d
exam2d_HC 1 1 C:\Bio guest - hmqcgpqf, HMQC Cyclosporin
exam1d_1H 1 1 C:\Bio guest - zg, 1H Cyclosporin

Figure 4.3

☞ Hit the ***Enter*** key to display the highlighted dataset in the current window

☞ Double-click a dataset to display it in the current window.



→ Remove the selected dataset from the list.
→ Open a dialog to select a *Last50* list.
→ Open a dialog for saving the current *Last50* list.

Figure 4.4

Each line displays one dataset showing its *name, expno, procno, top level directory* and *user.*

The Groups tab

Clicking the ***Groups*** tab displays the list of user defined dataset groups. Here you can create, modify and display groups of datasets. Defining a group is useful is you work on projects where each project involves multiple datasets. It allows you to easily organizes your projects and access all data belonging to a certain project.



→ Display selected dataset(s) in active window
→ Display selected dataset(s) in new window.
→ Display all datasets in group in new windows.
→ Add selected data window to selected group.
→ Add all open data windows to selected group.
→ Update window bounds and dislay regions.
→ Remove selected datasets from group.
→ Collapse all groups.
→ Show/hide dimension, pulse program, title.
→ Add a new (empty) dataset group to the list.
→ Close all data windows of selected group.
→ Process selected dataset with serial processing.
→ Show file properties of selected dataset.
→ Show file list of selected dataset.
→ Copy pathnames of selected data to clipboard.

Figure 4.5

Note that a group not only defines the datasets involved, but also their data window positions and dimensions and the displayed region of each spectrum.

The entry ***Update window bounds & display regions***

The Alias tab

Clicking the ***Alias*** tab displays the list of user defined alias names for datasets. Just right-click any entry to define, remove or interpret alias names.

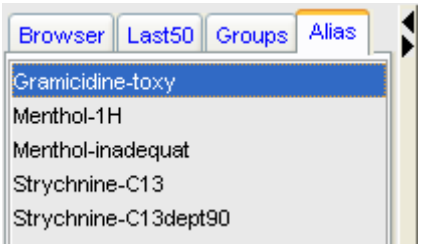
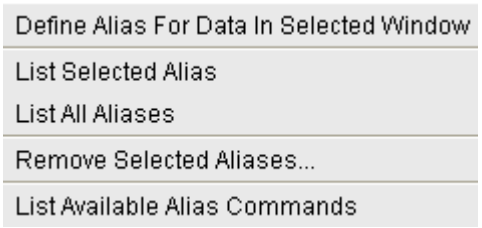


Figure 4.6


Define Alias For Data In Selected Window
List Selected Alias
List All Aliases
Remove Selected Aliases...
List Available Alias Commands

→ define alias for data in selected window.

→ Show selected data name, expno etc.

→ Show all data names, expnos etc.

→ Remove selected aliases from list.

→ Show available alias commands.

Figure 4.7

How to Open the Browser in a separate window

The browser can be opened in a separate window as follows:

☞ Click ***Options*** → ***Preferences*** [`set`], click ***Window settings*** and check ***Display dataset browser in a separate window***.

You must restart TOPSPIN for the change to take effect.

How to Put the Focus in the Browser

☞ Hit the ***F2*** key

or

☞ Click inside the browser

How to Select Folders in the Browser

To select a particular folder:

☞ Left-click the folder button

or

☞ Hit the arrow-up/down keys while the focus is in the browser

To select multiple folders:

☞ Hold the ***Ctrl*** key and left-click multiple folders to select them

or

☞ Hold the ***Shift*** key and left-click two folders to select these two and all in between.

How to Expand/Collapse a Folder in the Browser

To expand a collapsed folder:

☞ Click the + button to the left of the folder button

or Double-click the folder button

or Hit the ***Right-Arrow*** key while the folder is highlighted

To fully expand a collapsed folder:

☞ Right-click the DIR, NAME or EXPNO node and choose ***Fully Expand Selection***

To collapse an expanded folder:

☞ Click the - button to the left of the folder button

or Double-click the folder button

or Hit the ***Left-Arrow*** key while the folder is highlighted

How to Show/Hide Pulse program and Title in the browser

☞ Right-click the data name folder button and choose

Show PULPROG /Title from the popup menu (see Fig. 4.8)

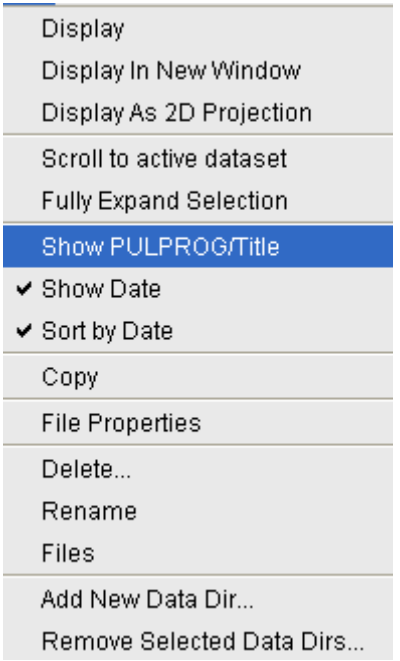


Figure 4.8

How to Show Dataset Dates in the Browser

☞ Right-click the data name folder button and choose ***Show Date***

The last modified date is shown to the right of the dataset NAME, whereas the acquisition date is shown to the right of the dataset EXPNO (see Fig. 4.9).

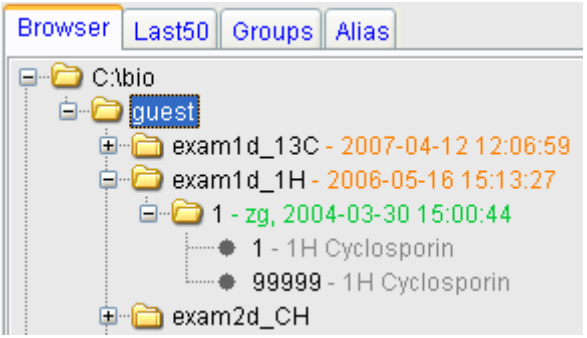


Figure 4.9

How to change the default Top Level Data Directory

By default, the browser shows the TOPSPIN installation directory with the Bruker example datasets. To suppress this feature click ***Options*** → ***Preferences*** [`set`], click ***Administration*** and uncheck ***Show TOPSPIN data examples directory in data browser***.

How to Add, Remove or Interpret Alias Names

To add an alias name:

1. Click the ***Alias*** tab in the browser.
2. Right-click in the Alias table to open the popup menu (see Fig. 4.7). Click ***Define alias names for data in selected window***.
3. Enter an alias name in the appearing dialog box and click ***OK***. Note that alias names must begin with a letter.

To remove an alias name:

1. Right-click the ***alias name***
2. Click ***Remove selected aliases...*** from the popup menu (see Fig. 4.7)

Furthermore, the popup menu offers entries to display the dataset, list its properties and print the full dataset specification.

4.2 Creating Data

How to Create a New Dataset

1. Click ***File*** → ***New*** [***new***, ***Ctrl***+***n***]

   or

   Click the button  in the upper toolbar.

2. Specify the dataset *name*, *expno*, *procno*, *dir*, and *user* in the appearing dialog box. If one or more datasets are open, the fields are initialized with the current dataset (see Fig. 4.10).
3. Click the down-arrow of the ***Solvent*** box and choose a solvent from the list, or type a solvent name.
4. Click the down-arrow of the ***Experiment*** box and choose a parameter set from the list, or type a parameter set name.
5. Type the dataset title in the ***TITLE*** box.
6. Click ***OK***.

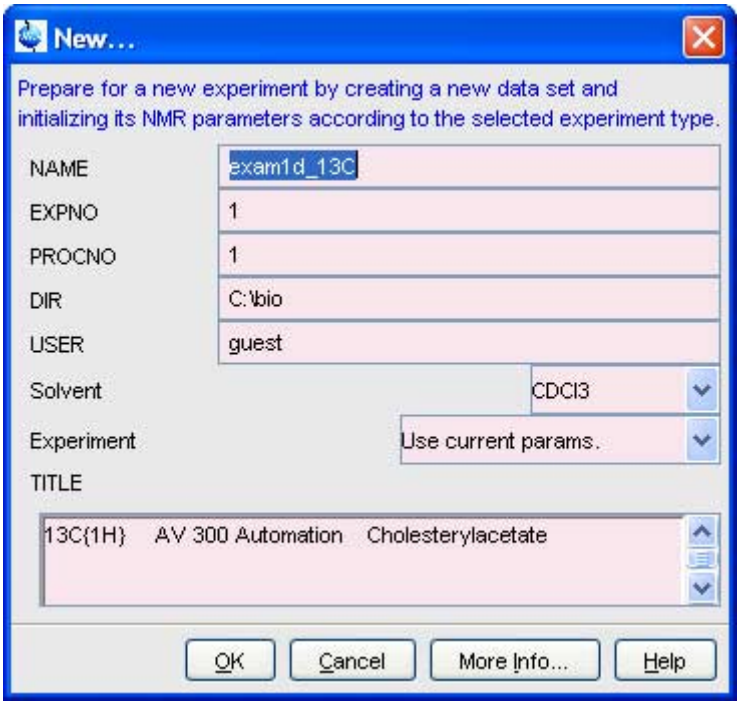


Figure 4.10

A dataset will be created and initialized with the parameters of the chosen experiment. No fid or spectrum are available yet. They can be created by data acquisition and data processing, respectively.

4.3 Opening Data

TOPSPIN allows you to open data in several ways, from the browser, the menu, the Windows Explorer or the command line. Furthermore, data can be opened:

- in an existing data window replacing the current dataset.
- in a data window which is in multiple display mode, being superimposed on the current spectra.
- in a new data window which becomes the active window.

Note that if a dataset is already displayed in one window and it is opened in a sec-

ond existing window, it still replaces the dataset in the latter one. As a result, the same dataset will be displayed in two windows (see also command ***reopen***).

How to Open Data Windows Cascaded

By default, a new data window appears maximized, filling the entire data field and covering possibly existing window. You can, however, configure TOPSPIN to open new windows cascaded. This is convenient if you want to open several data windows and then select one.

To open new windows cascaded:

1. Click ***Options*** → ***Preferences*** [***set***]
2. Click ***Window Setting*** in the left part of the dialog box.
   The right part of the dialog box shows the window settings (see Fig. 4.11).

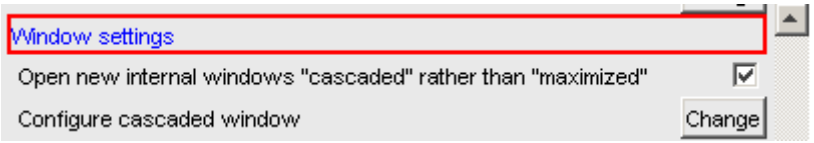


Figure 4.11

3. Check *Open new internal windows 'cascaded' rather than 'max'*.
4. Optionally you can configure the cascaded windows by clicking the respective ***Change*** button. This will open the dialog box shown in Fig. 4.12.

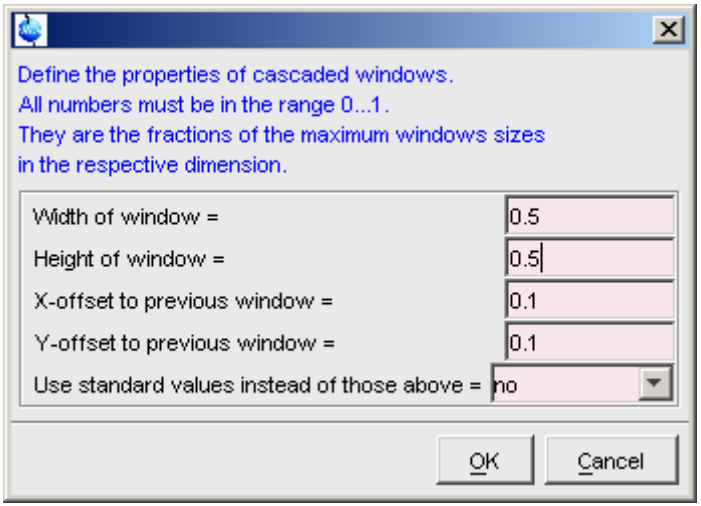


Figure 4.12

5. Here you can specify the data window sizes and offsets as fractions of the maximum window sizes.
6. Click ***OK*** to close the dialog box.

How to Open Data from the Browser

In the browser:

☞ Left-click-hold a data *name*, *expno* or *procno* and drag it into the data area. The data will be displayed in a new data window.

or Left-click-hold a data *name*, *expno* or *procno* and drag it into an open data window. The data will replace the currently displayed data.

or Left-click-hold a data *name*, *expno* or *procno* and drag it into an empty data window created with ***Alt+w n***.

or Left-click-hold a data *name*, *expno* or *procno* and drag it into a multiple display data window. The data will be superimposed on the currently displayed data.

or Right-click a data *name*, *expno* or *procno* and choose ***Display*** from the pop-up menu; the data will be displayed in the current data window.

or Right-click a data *name*, *expno* or *procno* and choose ***Display in new win-***

dow from the popup menu; the dataset will be displayed in a new data window.

or Hold the ***Ctrl*** key and left-click several datasets to select them or hold the ***Shift*** key and left-click two datasets to select these two and all in between. Then right-click one of the selected datasets and choose ***Display*** from the popup menu. A new window will be opened showing the selected datasets in multiple display mode. However, if the current window was already in multiple display mode, the selected spectra will be superimposed on the currently displayed spectra.

How to Automatically Select the first *expno*/*procno* of a dataset

If you open a dataset from the Browser by clicking a data *name*, there might be more that one *expno* and/or *procno* available. By default, TOPSPIN then opens a dialog box from which you can select the desired *expno/procno* combination (see Fig. 4.13). Clicking ***Open*** will open the selected dataset, whereas clicking ***Print*** will print the displayed dataset list.

You can, however configure TOPSPIN to automatically open the first available *expno*/*procno* combination. To do that:

1. Click ***Options*** → ***Preferences*** [***set***].
2. Click ***Miscellaneous*** in the left part of the dialog box.
3. Uncheck the item *Display EXPNO/PROCNO list when opening data*.
4. Click ***OK*** to close the dialog box.

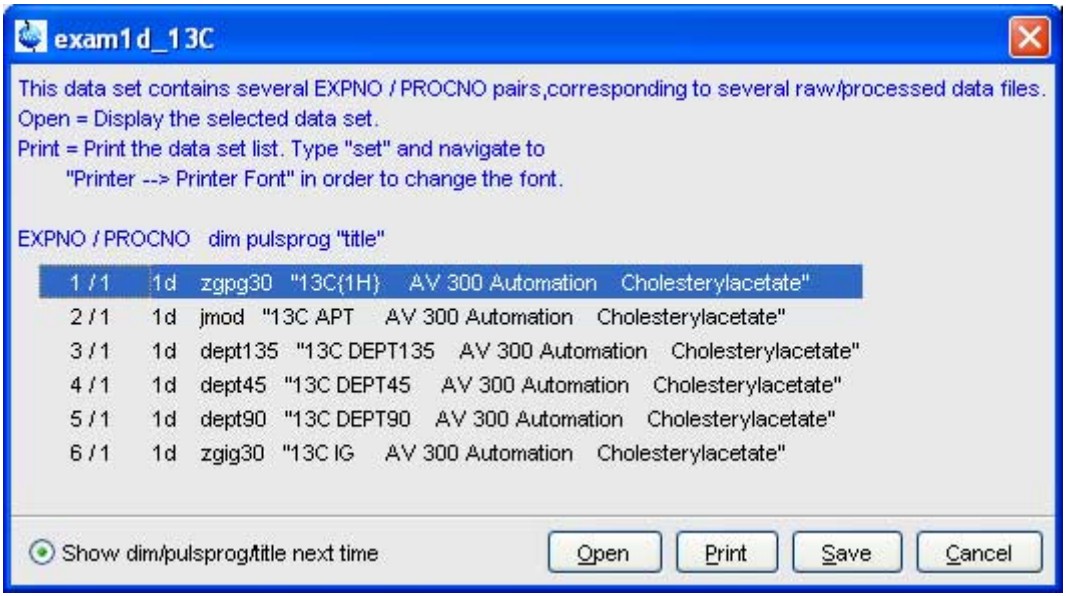

exam1 d_13C
This data set contains several EXPNO / PROCNO pairs,corresponding to several raw/processed data files.
Open = Display the selected data set.
Print = Print the data set list. Type "set" and navigate to
"Printer --> Printer Font" in order to change the font.
EXPNO / PROCNO dim pulsprog "title"
1 / 1 1d zgpg30 "13C{1H} AV 300 Automation Cholesterylacetate"
2 / 1 1d jmod "13C APT AV 300 Automation Cholesterylacetate"
3 / 1 1d dept135 "13C DEPT135 AV 300 Automation Cholesterylacetate"
4 / 1 1d dept45 "13C DEPT45 AV 300 Automation Cholesterylacetate"
5 / 1 1d dept90 "13C DEPT90 AV 300 Automation Cholesterylacetate"
6 / 1 1d zgig30 "13C IG AV 300 Automation Cholesterylacetate"
Show dim/pulsprog/title next time
Open
Print
Save
Cancel

Figure 4.13

Note that the command ***rel*** also opens the dialog shown in Fig. 4.13, showing the available EXPNO's under the current dataset. Similarly, ***repl*** shows the available PROCNO's under the current dataset EXPNO.

How to Open Data from the Topspin menu

1. To open a dataset:

   ☞ Click the  button in the upper toolbar.

   or

   ☞ Click ***File*** → ***Open*** [***open***, ***Ctrl+o***] (see Fig. 4.14).



Figure 4.14

2. In the appearing dialog box (see Fig. 4.15)

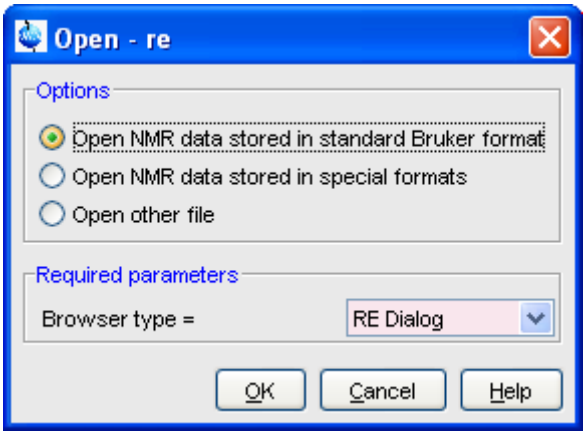


Figure 4.15

a) Select the option ***Open NMR data stored in standard Bruker format***.

b) Select the browser type ***RE Dialog***.

c) Click ***OK***.

3. In the appearing dialog box (see Fig. 4.16).

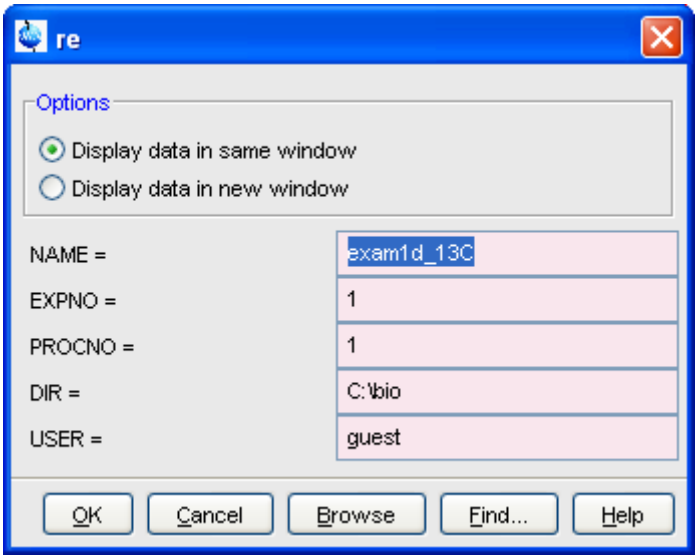


Figure 4.16

a) Specify the dataset *name*, *expno* etc.

b) Click ***OK***.

Note that the dataset specification consists of the five variable parts of the data directory tree, in this case:

C:\bio\data**guest**\nmr**exam1d_1H\1**\pdata**1**

The text boxes are initialized with the dataset in the current data window.

How to Open Data from the Explorer, Konqueror or Nautilus

You can open a dataset from the Windows Explorer as follows:

1. Open the Windows Explorer. You can do that in two different ways:

   ☞ from the Windows ***Start*** button. Navigate to the data *name*, *expno* or *procno*.

   or

   ☞ by entering the command ***expl*** in TOPSPIN. The Explorer shows the contents of the current dataset *procno* directory. Navigate to the desired data

name, *expno* or *procno*. ***expl*** can also be used with the argument ***top*** to open the TOPSPIN installation directory, ***home*** to open user home directory or with an absolute pathname to open that directory.

2. Now you can open a dataset with:

   ☞ **drag & drop**: click-hold a dataset *name* or any of its sub-folders or files and drag it into the TOPSPIN data area or data window.

   or

   ☞ **copy & paste**: right-click a dataset and choose ***copy*** from the popup menu. In TOPSPIN, click ***Edit*** → ***Paste*** [***paste***] (see Fig. 4.17).

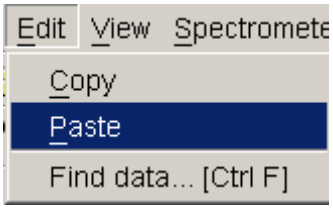


Figure 4.17

Likewise, a dataset can be opened from the Windows

window or Internet Browser.

How to Open Data from the Command Line

To open a dataset from the command line:

1. Enter ***re***
2. Specify a dataset in the appearing dialog box (see Fig. 4.16).
3. Click ***OK***

To open a new *procno* of the current dataset:

1. Enter ***rep***
2. Specify a *procno* in the appearing dialog box.
3. Click ***OK***

To open a dataset in a new window:

1. Enter ***rew***
2. Specify a dataset in the appearing dialog box.

3. Click ***OK***

To open a new *procno* of the current dataset in a new window:

1. Enter ***repw***
2. Specify a *procno* in the appearing dialog box.
3. Click ***OK***

To open a data browser and read a dataset from there:

1. Enter ***reb***
2. Select a dataset from the appearing dialog box.
3. Click ***Display***

Note that ***re***, ***rep*** and ***reb***:

- Replace the data in the currently selected data window.
- Open the data in a new window when they are used after typing ***Alt***+***w n***
- Add the data in the currently selected window if this is in multiple display mode.

whereas ***rew*** and ***repw*** :

- Always open the dataset in a new window.

Topspin 2.0 and newer allows opening datasets stored in the following directories structures:

<mydata>/<dataname>/<expno>/pdata/<procno>

To do that

☞ Enter ***reb*** on the command line, browse to the desired dataset and click the Display button

or

☞ Open the Operating System File Browser, browse to the desired dataset and open it in Topspin with **Copy & Paste** or **Drag & Drop**.

Note that this will create a copy of the dataset in the standard Topspin datapath:

<tshome>/data/<user>/nmr/<dataname>/<expno>/pdata/<procno>

where <user> is the current internal Topspin user. This copy can be processed, deleted or overwritten, even if the original dataset is write protected. The origi-

nal data set is left unchanged.

How to Open Special Format Data

Apart from the standard Bruker data format, TOPSPIN is able to read and display various other formats. To do this:

☞ Click ***File*** → ***Open*** [**`open`**, **`Ctrl`**+**`o`**]

select the option ***Open NMR data stored in special formats***, select the desired file type (see Fig. 4.18) and click **`OK`**.

A dialog will appear which depends on the chosen file type. Just follow the instructions on the screen.

The following file types are supported:

- JCAMP-DX - Bruker TOPSPIN[1] data stored in JCAMP-DX format
- Zipped TOPSPIN - Bruker TOPSPIN data stored in ZIP format
- WINNMR - Bruker WINNMR data
- A3000 - Bruker Aspect 3000 data
- VNMR - data acquired on a Varian spectrometer
- JNMR - data acquired on a Jeol spectrometer
- Felix - 1D data, FID or spectrum, which are stored in FELIX format.

Note that in all cases, the data are stored in a single data file which is unpacked/converted to standard Bruker format, i.e. to a data directory tree.

1. Note that the TOPSPIN data format is identical to the XWIN-NMR data format.

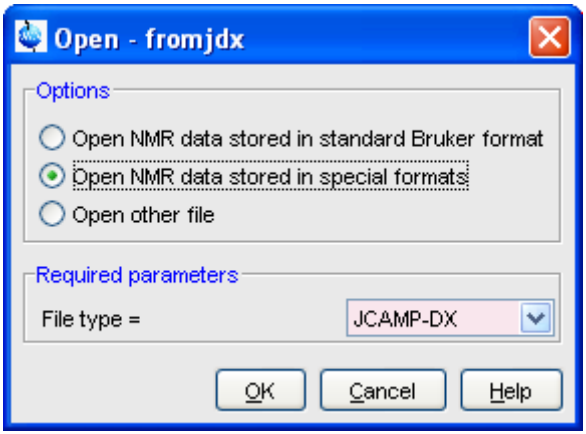


Figure 4.18

How to Open a ZIP or JCAMP-DX file from the Windows Explorer

Data stored in ZIP or JCAMP-DX format can also be opened directly from the Windows Explorer. You can do that in one of the tree following ways:

Drag & drop

☞ Click-hold a file with the extension `.dx` or `.zip` and drag it into the TOPSPIN data area or data window.

Copy & paste

1. Right-click a file with the extension `.dx` or `.zip` and choose ***copy*** from the popup menu.
2. In TOPSPIN, click ***Edit*** → ***Paste*** [***paste***]

Associate JCAMP-DX files with a script

1. Create a file with the extension `.cmd` (e.g. `jcamp.cmd`) with a text editor.
2. Enter the following line :

   ```
   <tshome>\prog\bin\sendgui.cmd fromjdx %1
   ```

   and store the file.
3. Open the Explorer and find the JCAMP-DX file.
4. Right-click the filename and choose ***Open with*** → ***Choose program*** →

Browse

5. Find and select the script and click ***OK***.

Now, every file with the extension .dx will automatically be opened in TOPSPIN when double clicked.

4.4 Saving/Copying Data

How to Save or Copy Data

You can save the current dataset as follows:

1. Click ***File*** → ***Save*** [***Ctrl***+***s***].

   This will open a dialog box (see Fig. 4.19).

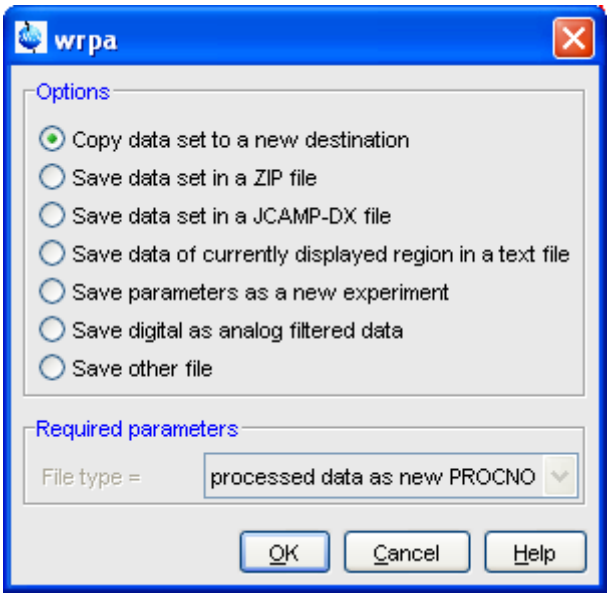

wrpa
Options
Copy data set to a new destination
Save data set in a ZIP file
Save data set in a JCAMP-DX file
Save data of currently displayed region in a text file
Save parameters as a new experiment
Save digital as analog filtered data
Save other file
Required parameters
File type =
processed data as new PROCNO
OK
Cancel
Help

Figure 4.19

2. Select an option and, if applicable, a file type.
3. Click ***OK*** to execute the option.

The six options correspond to the following command line commands:

- ***wrpa*** - copies the current data to a new data *name* or *expno*
- ***tozip*** - convert a dataset of any dimension to ZIP format
- ***tojdx*** - convert a 1D or 2D dataset to JCAMP-DX format
- ***totxt*** - convert a 1D or 2D dataset text format
- ***wpar*** - write parameter set
- ***convdta*** - save digitally filtered data as analog filtered data
- ***wrp***, ***wra***, ***genfid***, ***wmisc*** - write various files

How to Save an Entire Dataset

1. Click ***File*** → ***Save*** [***Ctrl***+***s***].
2. Select the option ***Copy dataset to a new destination*** [***wrpa***] and click ***OK***
3. Specify the dataset variables and click ***OK***

How to Save Processed Data

1. Click ***File*** → ***Save*** [***Ctrl***+***s***].
2. Select the option ***Save other file***
3. Select File type ***Processed data as new procno*** [***wrp***] and click ***OK***
4. Enter a processing number (*procno*) and click ***OK***

How to Save Acquisition Data

1. Click ***File*** → ***Save*** [***Ctrl***+***s***].
2. Select the option ***Save other file***
3. Select File type ***Acqu. data as new expno*** [***wra***] and click ***OK***
4. Enter a experiment number (*expno*) and click ***OK***

How to Save Processed Data as Pseudo Raw Data

1. Click ***File*** → ***Save*** [***Ctrl***+***s***]
2. Select the option ***Save other file***
3. Select File type ***1r/1i as fid*** [***genfid***] or ***2rr/2ii as ser*** [***genser***]
4. Click ***OK***
5. Enter a destination *expno.*

(optionally, you can specify further data path specifications)

6. Click ***OK***

4.5 Deleting Data

How to Delete a Specific Dataset

☞ Right-click the data *name*, *expno* or *procno* in the browser, then click ***Delete...***

A confirmation dialog will appear. Just click ***OK***, if you are sure you want to delete. Note that TOPSPIN does not allow you to delete the last available dataset, e.g. the last *procno* under an *expno*, the last *expno* under a *name* or the last *name* under a *user.*

How to Delete Types of Datasets

To delete certain types of data like 1D raw data, 2D processed data etc.:

☞ Click ***File*** → ***Delete...***

or

☞ Enter **`delete`** on the command line.

The dialog window shown in Fig. 4.20 will appear. Here you can select the data type and selection criteria.

4.6 Renaming Data

How to Rename a Specific Dataset

1. Right-click the data *name*, *expno* or *procno* in the browser, then click ***Rename...***
2. In the appearing dialog:
   Enter the new *name*, *expno* or *procno*
3. Click ***OK***

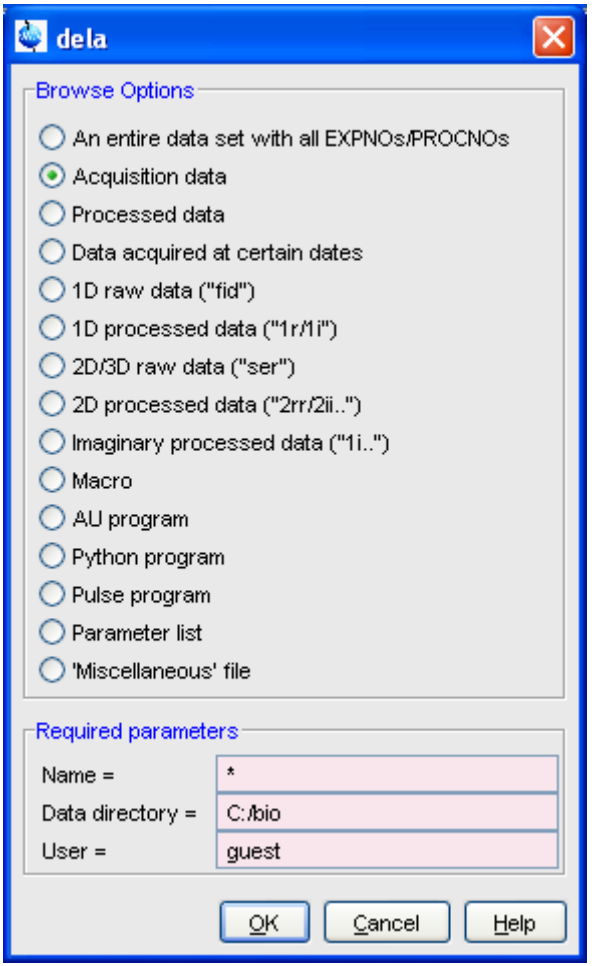


Figure 4.20

1. Select a data type option

   For each option, the corresponding command appears in the title of the dialog box. These commands can also be used to delete data from the command line.

2. Specify the ***Required parameters***

   Note that you can use the wildcards:

   - Asterix (*) for any character and any number of characters.

- Question mark (?) for any single character.

3. Click ***OK***

A dialog box will appear showing the matching datasets. For example, if you select the option ***An entire dataset ...*** :

1. Select dataset entries for deletion (selected entries are highlighted).

   To select multiple entries: click them holding the ***`Shift`*** or ***`Ctrl`*** key.

2. Click ***Delete*** to delete the entire data directory.

If you select the option ***Acquisition data*** or ***Processed data***, you can choose between deleting the data files only and deleting the entire *expno* or *procno* directory, respectively (see Fig. 4.21).

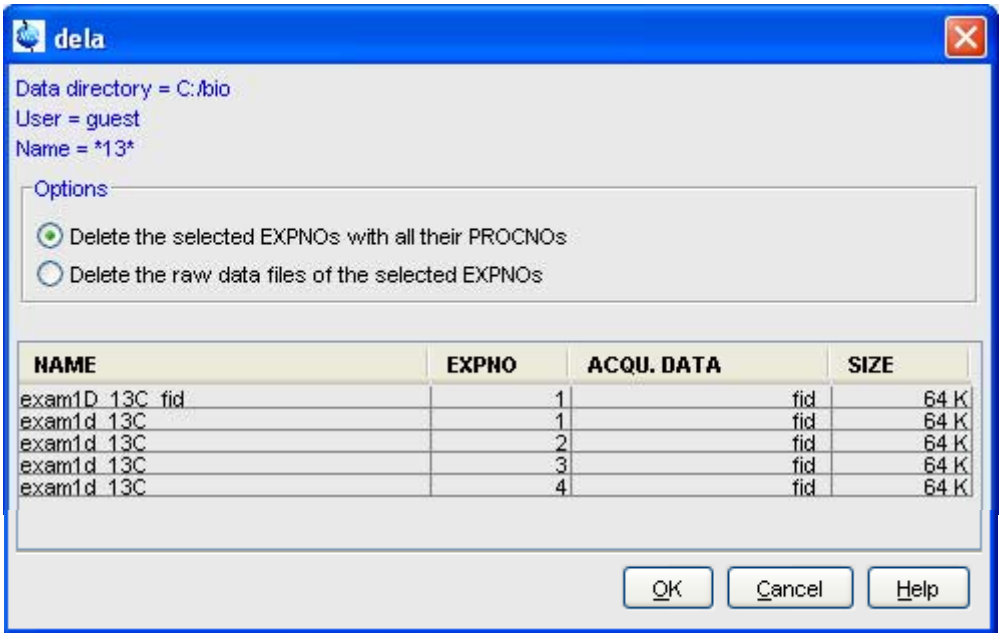


Figure 4.21

4.7 Searching/Finding Data

How to Find Data

You can find TOPSPIN data according to various criteria. To start searching, do the following:

1. Click ***Edit*** → ***Find data*** [**`Ctrl+f`** | **`find`**]
   to open the *Find data* window (see Fig. 4.22).

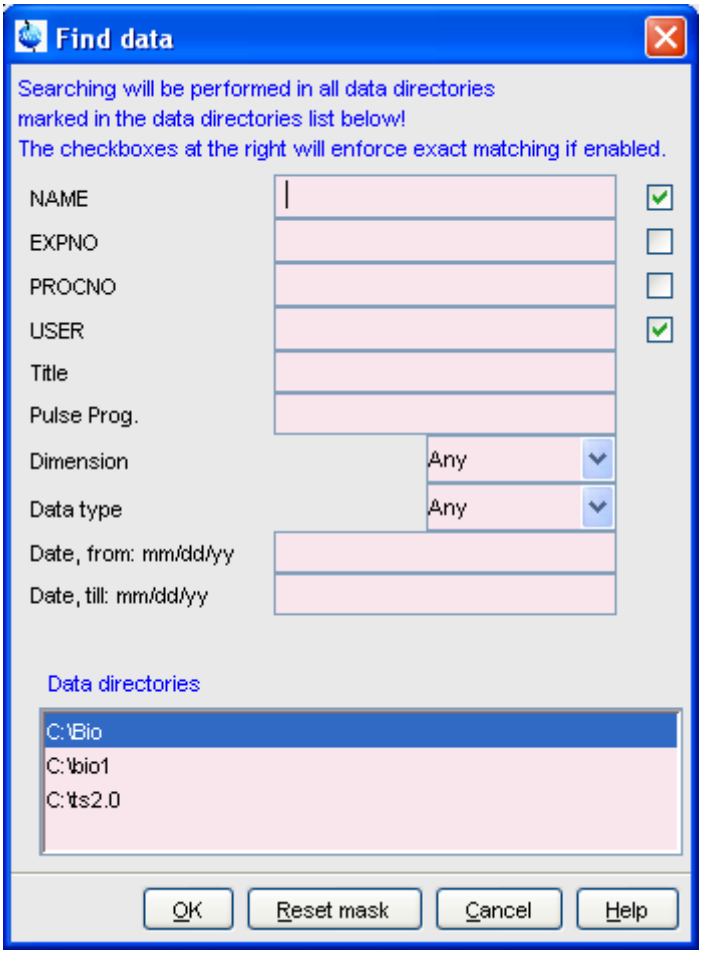


Figure 4.22

2. Enter the search items in the upper part of the dialog. Note that:
   - There will be searched for items containing the specified string
   - Exact matching is performed for dataset variables, NAME, EXPNO, PROCNO and USER, if the checkboxes at the right are enabled.
   - The search is restricted to data created between the specified dates. Note that this refers to the acquisition date.
   - The ***Reset mask*** button allows you to reset the default criteria.
3. Select the **Data directories** to be searched in the lower part of the dialog. If no directories are selected, all will be searched.
4. Click ***OK***
   to start the search. A list of data that fulfil the defined criteria will appear (see Fig. 4.23).

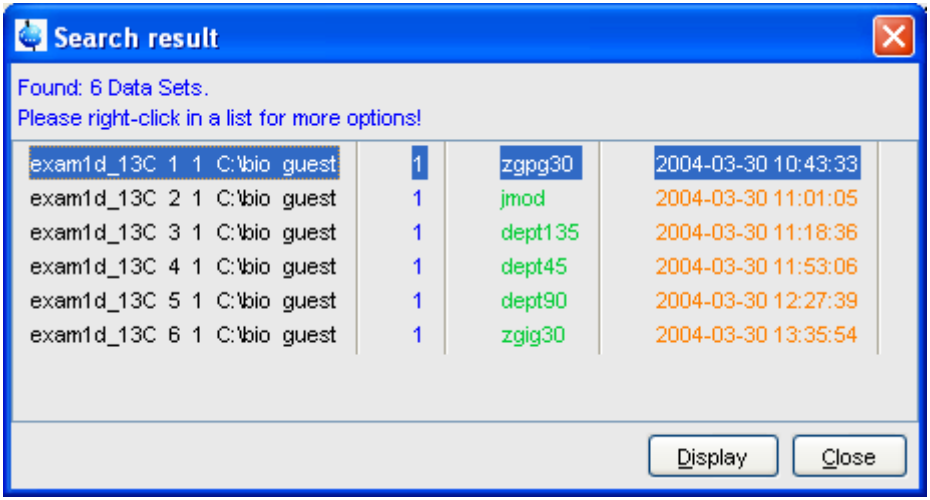

Search result
Found: 6 Data Sets.
Please right-click in a list for more options!
exam1d_13C 1 1 C:\bio guest 1 zgpg30 2004-03-30 10:43:33
exam1d_13C 2 1 C:\bio guest 1 jmod 2004-03-30 11:01:05
exam1d_13C 3 1 C:\bio guest 1 dept135 2004-03-30 11:18:36
exam1d_13C 4 1 C:\bio guest 1 dept45 2004-03-30 11:53:06
exam1d_13C 5 1 C:\bio guest 1 dept90 2004-03-30 12:27:39
exam1d_13C 6 1 C:\bio guest 1 zgig30 2004-03-30 13:35:54
Display
Close

Figure 4.23

Note that on exiting TOPSPIN, the search criteria will be rest to default.

How to Display one of the Found Datasets

In the search result window (see Fig. 4.23):

1. Click one or more datasets to select them.
2. Click ***Display***

to display the selected dataset(s) in the current data window. If multiple datasets are selected they are displayed in the new data window in multiple display mode.

The search result window offers a right-click context menu with various options (see Fig. 4.24) .

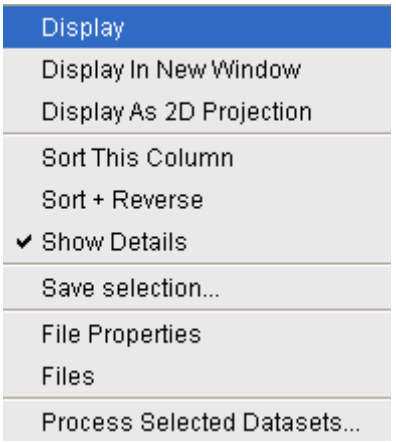


Figure 4.24

Display

Display the selected dataset(s) in the current data window. If multiple datasets are selected they are displayed in the same data window in multiple display mode. Equivalent to clicking the ***Display*** button or pressing ***Enter***.

Display In New Window

Display the selected dataset(s) in a new window. If multiple datasets are selected they are displayed in the one new data window in multiple display mode.

Display As 2D Projection

Display the selected dataset as a projection of the current 2D dataset. A dialog will appear allowing you to choose F1-projection, F2-projection or both. If multiple datasets are selected, only the first one is considered. If the current dataset is not a 2D dataset, nothing happens.

Sort This Column

Sort the selected column in ascending order.

Sort + Reverse

Sort the selected column in descending order.

Save Selection

Save the list of selected datasets in a text file. First opens a file dialog where you can select or specify a filename. The saved dataset list can, for example, be used for serial processing (command ***serial***, see also ***Process Selected Datasets*** below).

File properties

Show main dataset parameters like *Dimension*, *Pulse program*, *Acquisition Date*, *Nuclei*, *Spectrometer frequency* and *Solvent*.

Files

Show the files in the processed data directory of the selected dataset.

Process Selected Datasets

Perform serial processing on the selected datasets. Opens a dialog where you can change or edit the dataset list and specify the command, macro or Python program to be executed (starts the command ***serial***).

The ***Close*** button allows you to close the search result dialog.

4.8 Handling Data Files

How to List/Open the Current Dataset Files

A Bruker dataset is represented by a directory tree which contains files in the *expno* and *procno* subdirectories. These files contain the actual data, parameters, lists etc.

☞ Right-click inside the data window and choose ***Files*** from the popup menu.



If the spectrum is displayed, the files in the *procno* subdirectory are shown. If the **Fid** is displayed, the files in the *expno* subdirectory are shown.

☞ Select a file and click ***Open*** to view its contents.

Note that this only makes sense for ascii files.

How to List/Open the current Dataset Files in the Windows Explorer

To list the current dataset files in the Windows Explorer:

1. Click ***Files*** → ***Run...***
2. Select ***Open file explorer*** [***expl***] in the appearing dialog box (see Fig. 4.25)
3. Click ***OK***

Alternatively, you can enter the command ***expl*** on the command line.The Windows Explorer will be opened showing the processed data files (the files in the *procno* directory) of the current dataset. Under Linux a Web browser like KDE Konqueror or Gnome Mozilla will be opened.

To open a file:

☞ Double-click the file or right-click the folder icon and choose ***Open***

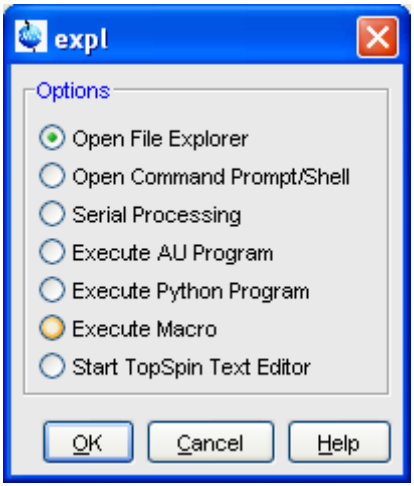


Figure 4.25

If TOPSPIN data area contains no datasets, the ***expl*** command opens the Explorer showing the users home directory. When entered on the command line, ***expl*** can also be used with the argument ***top*** to open the TOPSPIN installation directory, ***home*** to open user home directory or with an absolute pathname to open that directory.

Chapter 5

Parameter Handling

5.1 Processing Parameters

Processing parameters can be set/changed in three different ways:

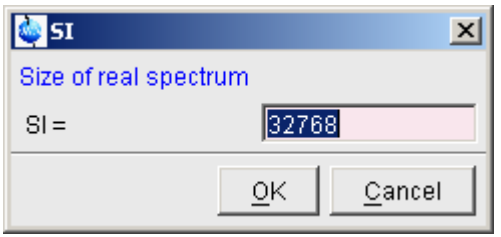
- from the parameter editor: click the ***ProcPars*** tab or enter ***edp***
- from the command line: e.g. enter ***si***
- from a command dialog box: e.g. ***wm***

How to Set a Processing Parameter from the Command Line

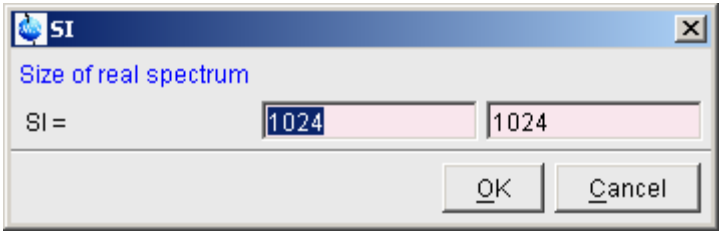
Enter the parameter name on the command line. For example to set the size:

1. Enter ***si***

   for 1D data, the following dialog box will appear:



for 2D data, the following dialog box will appear:



2. Specify the desired value(s), e.g. **32768** or **32k**
3. Click ***OK***

How to Set Processing Parameters from the Parameter Editor

To open the processing parameter editor:

☞ Click the ***ProcPars*** tab in the Tab bar of the data window.

or

☞ Enter ***edp*** on the command line.

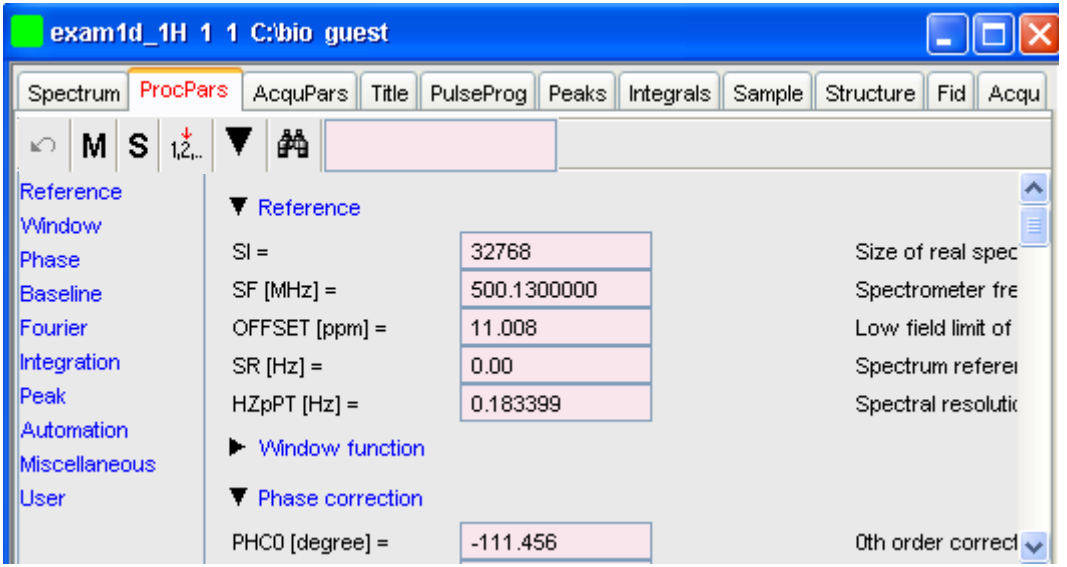


Figure 5.1

At the left of the parameter editor window you will see a list of parameter sections.

The processing parameter editor supports the following functions:

- ☞ Collapse/expand a parameter section by clicking the ▼ button. Note that the section Window function in Fig. 5.1 is collapsed.
- ☞ Collapse/expand all parameter sections by clicking the large ▼ button of the data window toolbar.
- ☞ Enter (part of) a parameter name in the search field and click 🔭 .
- ☞ Click a parameter section, e.g. Phase at the left of the dialog box. The section becomes highlighted and the corresponding parameters will appear in the right part of the dialog box.
- ☞ Click in a parameter field, e.g. PHC0, to set the parameter value.
- ☞ Click the [...] button to the right of parameters like AUNMP to open a list of the corresponding programs/lists.
- ☞ Right-click the [E] button to the right of parameters like AUNMP to open the current program/list with an editor.
- ☞ Hit the ***Tab*** key to jump to the next parameter field.
- ☞ Hit ***Shift***+***Tab*** to jump to the previous parameter field.
- ☞ Use the scroll bar at the right of the dialog box to move to parameters further up or down in the dialog box.

How to Undo the Last Processing Parameter Change

☞ Click the following button:

↶ Undo last parameter change.

How to Display Processing Status Parameters

☞ Click the following button:

S Show processing status parameters.

Note that the command ***dpp*** opens the parameter editor and automatically shows the status parameters.

How to Switch to Maxent parameters

☞ Click the following button:


Switch to Maxent parameters.

How to Change Processed Data Dimensionality

☞ Click the following button:


Change data dimensionality.

This changes the number of parameter columns and value of the processing parameter PPARMOD. TOPSPIN 2.1 and newer support data dimensionalities up to 8D.

The parameter editor does not allow you to modify status parameters. Processing status parameters reflect the status of the processed data and are used for further processing, display or plotting. Changing them can make the dataset inconsistent. In rare cases, however, it can be useful to change a status parameter and TOPSPIN allows you to do that from the command line. If, for instance, you want to change the F1 status parameter MC2 of a 2D dataset, you have to enter:

```
s mc2
```

Note that the command ***s*** is used for 1D, 2D and 3D dataset. TOPSPIN automatically recognizes the dimensionality of the data and displays the parameter in all relevant dimensions. Note that, for example, the parameter MC2 only exists in F1.

5.2 Acquisition Parameters

How to Set Acquisition Parameters

Acquisition parameters can be set/changed as follows:

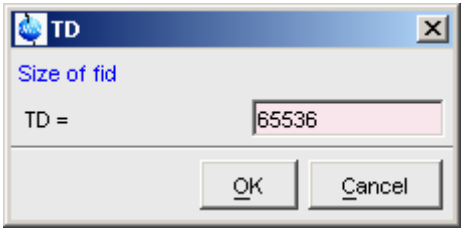
- from the parameter editor: click the ***AcquPars*** tab or enter ***eda***
- from the command line: e.g. enter ***td***
- from the interactive parameter adjustment window (enter ***gs***)

How to Set an Acquisition Parameter from the Command Line

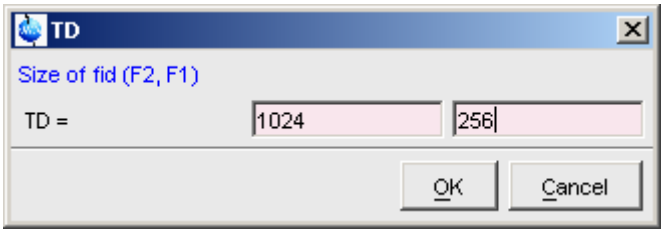
Enter the parameter name on the command line. For example to set the time domain size:

1. Enter ***td***

   for 1D data, the following dialog box will appear:



   for 2D data, the following dialog box will appear:



2. Specify the desired value(s), e.g. **65536** or **64k**
3. Click ***OK***

How to Set Acquisition Parameters from the Parameter Editor

To open the acquisition parameter editor:

☞ Click the ***AcquPars*** tab in the Tab bar of the data window.

or

☞ Enter ***eda*** on the command line.

Fig. 5.2 shows an example of the acquisition parameter editor with the Experiment parameters displayed.

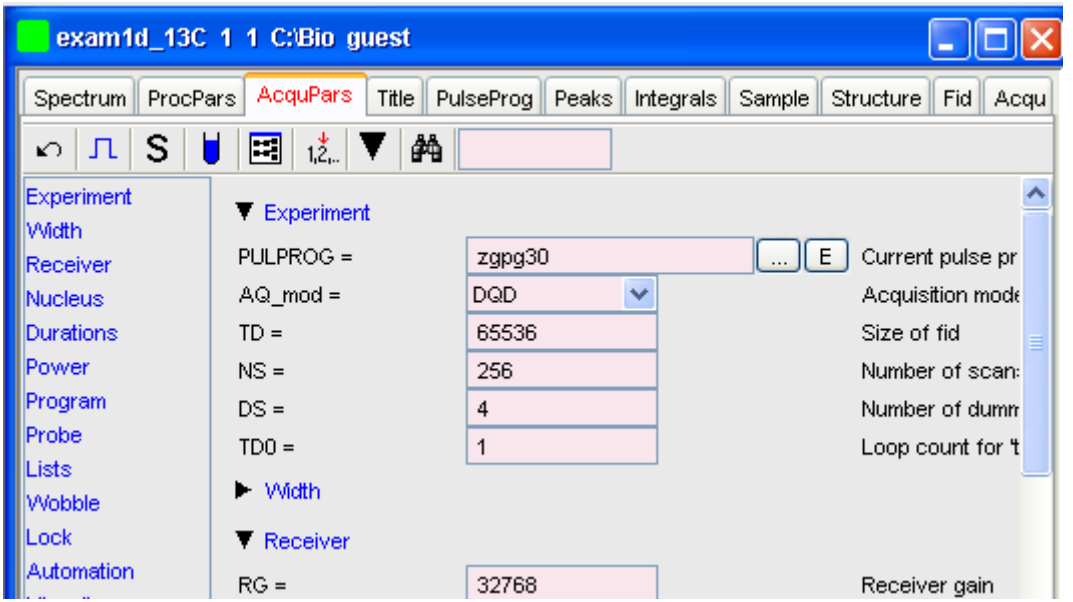


Figure 5.2

The processing parameter editor supports the following functions:

- ☞ Collapse/expand a parameter section by clicking the ▼ button. Note that the section Width in Fig. 5.2 is collapsed.
- ☞ Collapse/expand all parameter sections by clicking the large ▼ button of the data window toolbar.
- ☞ Enter (part of) a parameter name in the search field and click 🔭 .
- ☞ Click a parameter section, e.g. Experiment at the left of the dialog box. The section becomes highlighted and the corresponding parameters will appear in the right part of the dialog box.
- ☞ Click in a parameter field, e.g. TD, to set the parameter value.
- ☞ Click the … button to the right of parameters like PULPROG to open a list of the corresponding programs/lists.

☞ Right-click the E button to the right of parameters like PULPROG to open the current program/list with an editor.

☞ Hit the ***Tab*** key to jump to the next parameter field.

☞ Hit ***Shift***+***Tab*** to jump to the previous parameter field.

☞ Use the scroll bar at the right of the dialog box to move to parameters further up or down in the dialog box.

How to Undo the Last Acquisition Parameter Change

☞ Click the following button:

Undo last acquisition parameter change.

How to Set Pulse Program Parameters

☞ Click the following button:

Show pulse program parameters [***ased***]

The button will change to . To make this the default setting:

Click ***Options*** → ***Preferences***, click ***Miscellaneous***, check the entry "*Show ased parameter selection with eda*" and click ***OK***.

How to Display Acquisition Status Parameters

☞ Click the following button:

Show acquisition status parameters.

Note that the command ***dpa*** opens the acquisition parameter editor and automatically shows the status parameters.

How to Get Probehead/Solvent dependent Parameters

☞ Click the following button:

Set probehead/solvent dependant parameters [***getprosol***].

Probehead and solvent dependant parameters can be set up with the command ***edprosol***.

How to Change Acquisition Data Dimensionality

☞ Click the following button:



Change data dimensionality.

This changes the number of parameter columns and value of the acquisition parameter PARMODE.

How to Set Lock Parameters

Enter the command ***edlock*** and set the lock parameters in the appearing dialog box. For a detailed description of ***edlock***, please refer to the Acquisition Reference manual or enter ***edlock?*** on the command line.

How to Set Routing Parameters

Enter the command ***edasp*** and set the routing parameters in the appearing dialog box. For a detailed description of ***edasp***, please refer to the Acquisition Reference manual or enter ***edasp?*** on the command line.

Chapter 6

Data Processing

6.1 Interactive Processing

Interactive processing allows full control over the processing sequence. However, it requires detailed knowledge about the required parameters (see chapter 5.1) and commands. Therefore, it is only suitable for the advanced user. New or intermediate users are recommended to use the Processing Guide for semi-automatic processing (see chapter 6.2).

How to Process Data with Single Commands

Data can be processed by entering single commands on the command line. A typical 1D processing sequence would be:

- ***em*** : exponential window multiplication
- ***ft*** : Fourier transform
- ***apk*** : automatic phase correction
- ***sref*** : automatic calibration (referencing)
- ***abs*** : automatic baseline correction

This allows you full control over each individual processing step.

How to Process data with Composite Commands

Data can also be processed with so called composite commands. These are combinations of single processing commands. The following composite commands are available.

- ***ef*** : Exponential multiplication + Fourier transform
- ***efp*** : Exponential multiplication + Fourier transform + phase correction
- ***fmc*** : Fourier transform + magnitude calculation
- ***fp*** : Fourier transform +phase correction
- ***gf*** : Gaussian multiplication + Fourier transform
- ***gfp*** : Gaussian multiplication + Fourier transform + phase correction

They can be entered on the command line or clicked from the menu. For the latter option:

☞ Click ***Processing → More transforms → Shortcuts***

Just like single commands, composite commands can be used in Macros, AU programs and Python programs.

6.2 Semi-automatic Processing

How to Use the 1D Processing Dialog

1D data processing often involves the same sequence of steps, which can easily be performed as follows:

1. Click ***Processing → Process / Plot Current data***
2. In the appearing dialog (see Fig. 1.1):
   a) Enable the desired processing/plotting steps
   b) Set the parameter LB for exponential multiplication
   c) Select the desired LAYOUT for plotting.
   d) Click ***OK***

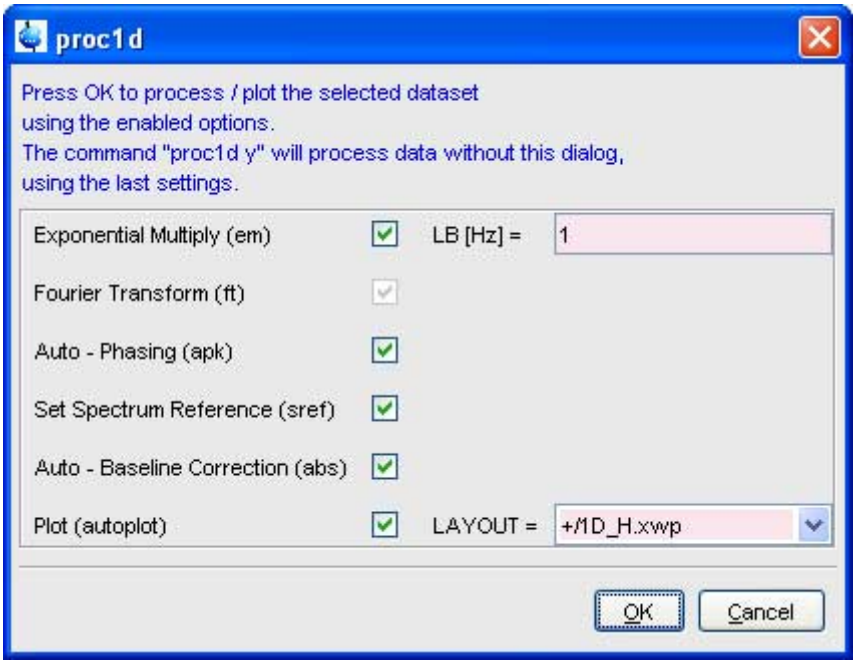


Figure 6.1

How to Use the Processing Guide in *Automatic* mode

The Processing Guide in automatic mode guides you through the entire processing sequence of data selection, processing, printing and archiving with minimum user interaction.

1. Click ***Processing → Processing Guide***

   The Processing Guide window will appear as an integral part of the current data window (see Fig. 6.2).

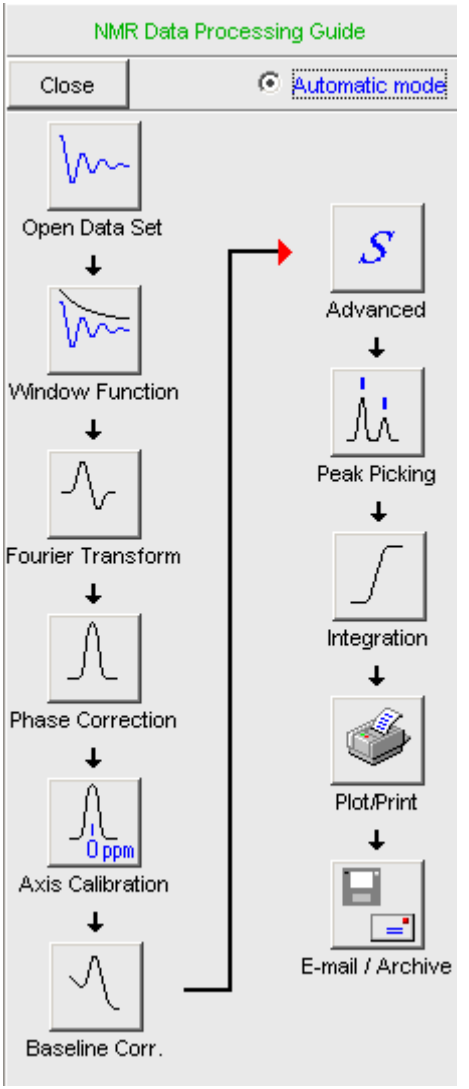


Figure 6.2

2. In the Processing Guide window:

a) Check ***Automatic mode***

b) Click ***Open data set*** and click ***OK*** to open a dataset manually, e.g. from the browser or click ***Browse*** to open the File Chooser.

c) Click ***Window function → Fourier Transform → etc.***

Each processing step will be executed without user interaction.

How to Use the Processing Guide in *Interactive* mode

The Processing Guide in interactive mode guides you through the entire processing sequence of data selection, processing, printing and archiving requiring some user interaction.

1. Click ***Processing → Processing Guide***

   The Processing Guide window will appear as an integral part of the current data window.

2. In the Processing Guide window:

   a) Uncheck ***Automatic mode***

   b) Click ***Open data set*** and click ***OK*** to open a dataset manually, e.g. from the browser or click ***Browse*** to open the File Chooser.

   c) Click ***Window function → Fourier Transform → etc.***

For each step a dialog box will appear where you can enter options, parameters etc. For details on these items, please refer to the corresponding commands in the Processing Reference Guide.

6.3 Processing Data with AU programs

Data processing can be performed by using AU programs. An AU program is actually a C-program which contains TOPSPIN commands (macros) and/or C-language statements. Various standard AU programs are delivered with TOPSPIN. A typical 1D processing AU program is ***proc_1d***. A simplified version of this AU program is:

```
EF
APK
SREF
ABS
AUTOPLOT
QUIT
```

It executes the commands ***ef***, ***apk***, ***sref***, ***abs*** and ***autoplot***. To run this AU

program, just enter ***proc_1d*** on the command line [1]. You can create your own AU programs with the command ***edau***. Note that an AU program must end with QUIT or QUITMSG("your message"), and that all statements must be specified in capital letters. For more information on AU programs, please refer to the AU programming manual:

☞ Click ***Help*** → ***Manuals*** → [**Programming Manuals**] ***AU Programming***

As an alternative to AU programs, you can also write Python programs, which allow you to use TOPSPIN commands, User Interface functions and Graphic functions. For more information:

☞ Click ***Help*** → ***Manuals*** → [**Programming Manuals**] ***Python Programming***

6.4 Serial Processing using Python programs

TOPSPIN allows you to process a series of datasets using serial scripts. The dataset list and command(s) to be used can be easily setup from the TOPSPIN interface as follows. Enter the command ***serial*** on the command line. This will open the

1. Before you can use any Bruker AU program, ***expinstall*** must have been executed once.

dialog window shown in Fig. 6.3.

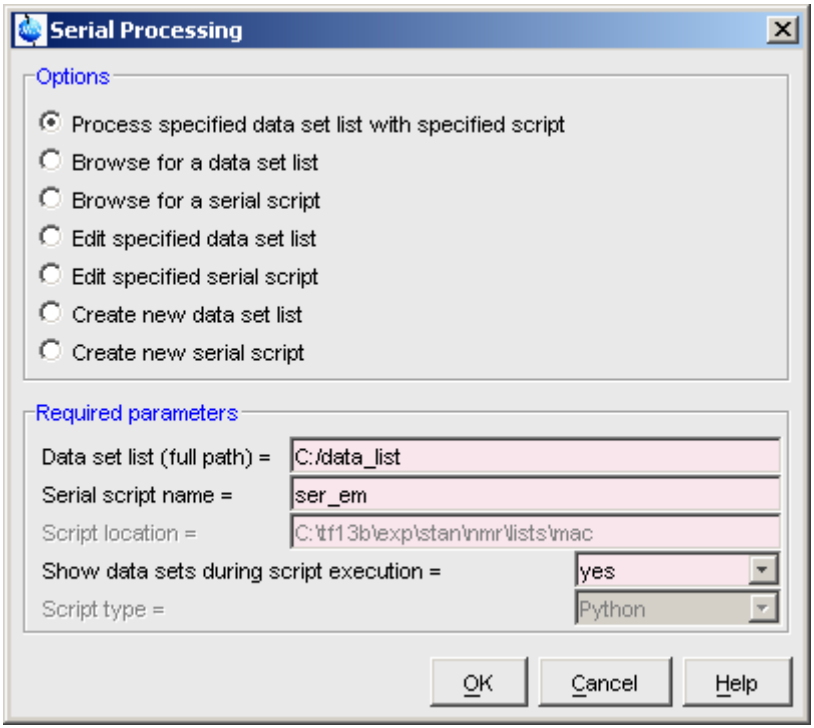


Figure 6.3

Here you can set up and start data processing of a series of datasets using scripts, which can be TOPSPIN macros or Python programs.

The dialog offers you the following options:

Process specified data set list with specified script

Process the data in the specified dataset list using the specified serial script. The flag ***Show data sets during script execution*** allows you to either display the currently processed dataset or remain on the current dataset.

Browse for a dataset list

Browse for an existing dataset list, starting in the users home directory.

Browse for a serial script

Browse for existing serial script. Depending on the parameter ***Script type***, the browser opens the ../exp/stan/nmr/py for ***Script type*** Python or ../exp/stan/nmr/lists/mac ***Script type*** macro. TOPSPIN, by default, searches for for files named `ser_*`.

Edit specified data set list

View or edit the list specified in the field ***Data Set List***.

Edit specified serial script

View or edit the script specified in the field ***Serial script name***

Create new data set list

Opens a dialog box for finding datasets. Proceed as follows:

1. Specify all search criteria and click ***OK***
2. In the appearing Search result box:
   a) Select the desired datasets.
   b) Click ***Save selection..***
3. In the appearing browser:
   a) Navigate to the desired list directory.
   b) Enter or select the list filename.
   c) Click ***OK***

Alternatively, you can create a dataset list manually.The format of a list entry is:

<name> <expno> <procno> <dir> <user>

An example of a dataset list is:

```
exam1d_13C 1 1 C:/bio guest
exam1d_13C 2 1 C:/bio guest
exam1d_13C 3 1 C:/bio guest
```

Alternatively, you can create a dataset list by specifying the absolute pathnames of a dataset, e.g.:

```
C:/bio/data/guest/nmr/exam1d_13C/1/pdata/1
```

Create new serial script

Opens the appropriate editor to create a new script. For ***Script type*** Python, ***edpy*** is executed, for ***Script type*** macro, ***edmac*** is executed. The name of a serial script (macro of Python) must start with `ser_`. Python scripts must have the extension `.py`. A standard example is the python script `ser_efp.py`.

An example of a simple processing sequence is exponential window multiplication, Fourier transform and automatic phase correction of a 1D dataset. A TOPSPIN macro performing this task would be:

```
ef

apk
```

A Python programs performing the same task would be:

```
EF()
APK()
```

Note that Python programs are much more versatile than macros. Details on Python programming can be found under:

☞ Click ***Help*** → ***Manuals*** → [**Programming Manuals**] ***Python Programming***

Note that serial processing can also be started as follows:

- Click ***Processing*** → ***Serial Processing...***

or

- Click ***File*** → ***Run***, select ***Execute Serial script on Data set list*** and click ***OK***

Chapter 7

Printing/Exporting Data

7.1 Printing/plotting Data

How to Print/Plot from the Menu

The current data window can be printed as follows:

1. From the TOPSPIN menu:

☞ Click the button  in the upper toolbar

or Click ***File*** → ***Print***

or Enter ***`print`*** or ***`Ctrl+p`***

All these actions are equivalent; they open the Print dialog box (see Fig. 7.1).

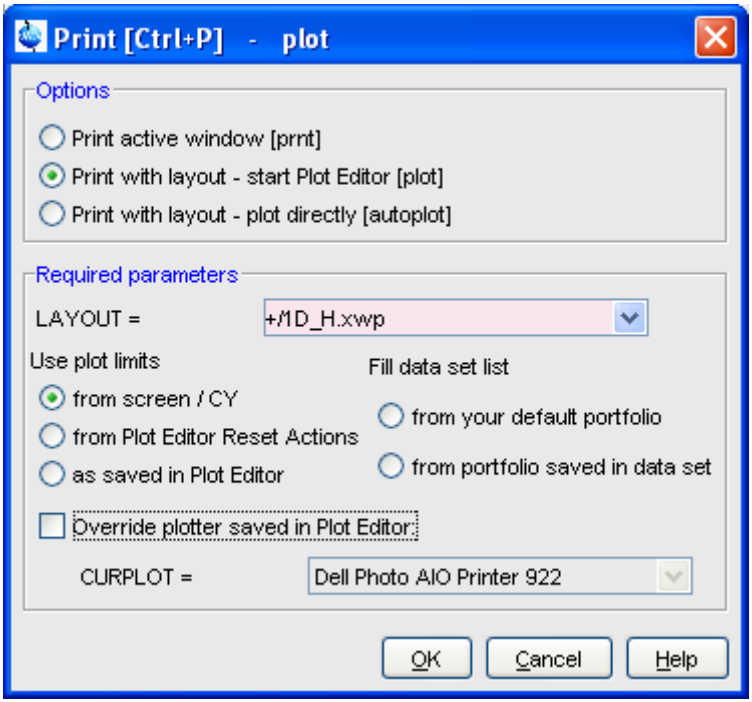


Figure 7.1

2. In the Print dialog box:

a) Select ***Print active window*** [**`prnt`**]

b) Click ***OK***

Before printing starts, the operating system print dialog box will appear. Here you can, for example, select the printer name and the printer properties.

The Print dialog box (see Fig. 7.1) contains two further options:

- ***Print with layout - start Plot Editor*** [**`plot`**]
  If you select this option and click ***OK***, the Plot Editor will be started. This option is equivalent to entering **`plot`** on the TOPSPIN command line.
- ***Print with layout - plot directly*** [**`autoplot`**]
  Selecting this option activates the Plot Editor layout list box. Select the desired layout and click ***OK*** to print. Standard layouts are delivered with TOPSPIN. They use the Windows default printer. User defined layouts use the

printer defined in the Plot Editor. On a 1D dataset, only 1D layouts are listed, on a 2D dataset only 2D layouts are listed etc.

For the last two options, the following Required Parameters are available:

Use plot limits

- ***from screen/ CY***
  The plot limits and maximum intensity are used as they are on the screen (processing parameter F1P, F2P and CY, respectively).
- ***from Plot Editor Reset Actions***
  The plot limits and maximum intensity are set according to the Plot Editor Reset Actions (right-click inside the Plot Editor data field and choose ***Automation*** to set the Reset Actions).
- ***as saved in Plot Editor***
  The plot limits and maximum intensity are set in the specified layout

Fill dataset list

- ***from your default portfolio***
  The portfolio contains the current TOPSPIN dataset plus the data from the default Plot Editor portfolio.
- ***from port folio saved in dataset***
  The portfolio contains the current TOPSPIN dataset plus the data from the portfolio stored in this dataset.

Override Plotter saved in Plot Editor

If enabled, the plotter defined in the Plot Editor layout will be overridden by de plotter defined by the processing parameter CURPLOT.

How to Plot Data from the Processing guide

Printing/plotting data can be done from the Processing guide by clicking the ***Plot/Print*** button. If ***Automatic mode*** is checked, the active data window will be printed as it appears in the screen. If ***Automatic mode*** is unchecked, you will get the dialog box as displayed in Fig. 7.1.

How to Plot Data with the Plot Editor

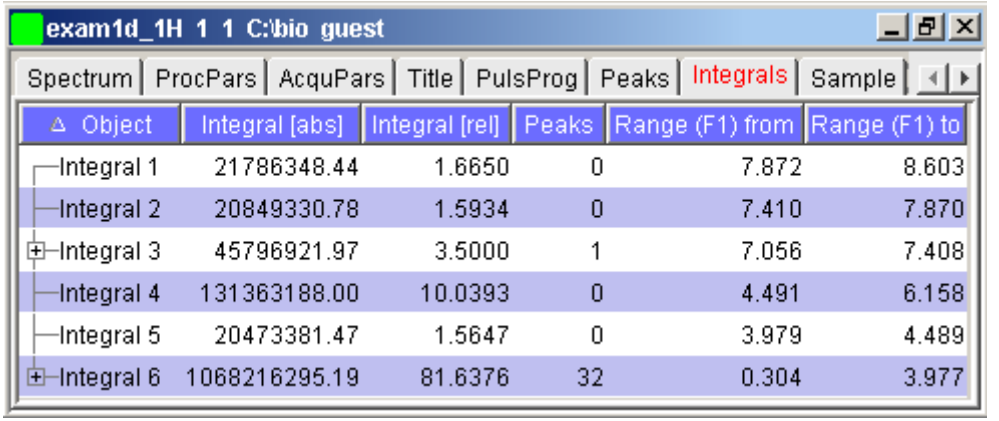
The Plot Editor can be started from the Plot Editor or from the command line (command ***`plot`***). The Plot Editor allows you to create layouts and plot data. The complete functionality is described in the online manual, which can be opened as

follows:

☞ Click ***Help*** → ***Manuals*** → [**Automation and Plotting**] ***TopSpin Plotting***

How to Print the Integral list

1. Click the ***Integrals*** tab of the data window (see Fig. 7.2).
2. Enter ***print*** or ***Ctrl+p*** to print it.



Object	Integral [abs]	Integral [rel]	Peaks	Range (F1) from	Range (F1) to
Integral 1	21786348.44	1.6650	0	7.872	8.603
Integral 2	20849330.78	1.5934	0	7.410	7.870
Integral 3	45796921.97	3.5000	1	7.056	7.408
Integral 4	131363188.00	10.0393	0	4.491	6.158
Integral 5	20473381.47	1.5647	0	3.979	4.489
Integral 6	1068216295.19	81.6376	32	0.304	3.977

Figure 7.2

How to Print the Peak list

1. Click the ***Peaks*** tab of the data window (see Fig. 7.3).
2. Enter ***print*** or ***Ctrl+p***



Figure 7.3

7.2 Exporting Data

How to Copy data to Other Applications

Under MS Windows, you can easily copy the data window contents to other applications. To do that:

☞ Click ***Edit*** → ***Copy*** [`copy`].

This will copy the data window contents to:

- the clipboard. After that you can paste the clipboard contents to any Windows application.
- the Windows Metafile file `screenDump.wmf` in the user properties directory (enter `hist` to locate this directory). The Windows Metafile can be imported by other applications or send to a different computer.

Please note:

Some programs, when importing spectra from the clipboard or metafile, do not display the contained information correctly. Particularly when you resize the imported graphics, sections of the text, the spectrum, or the axis sometimes have disappeared. Usually this is only a display problem. When you print the respective page, the representation is correct.

How to Store (Export) a Data Window as Graphics File

The clipboard and metafile formats are resizable vector formats. In addition to this, TOPSPIN allows you to save the contents of a data window in a graphics file of selectable type. Supported formats are .png, .jpg, .jpeg, .bmp, .emf, .wmf and .pdf. To do that:

1. Click ***File*** → ***Export***.... [***exportfile***].
2. Navigate to the storage folder.
3. Enter the destination filename and extension.
4. Click ***Export***

The resolution of such a *screen dump* equals the resolution of your screen.When you import a graphics file into an other program, you may loose information when resizing the graphics.

Note that exporting a data window to PDF-format is only supported in TOPSPIN 2.1 and newer.

Chapter 8

1D Display

8.1 The 1D Data Window

The 1D data window consists of a data field, a title bar, a Tab bar and buttons. Fig. 8.1 shows a data window with a 1D spectrum.

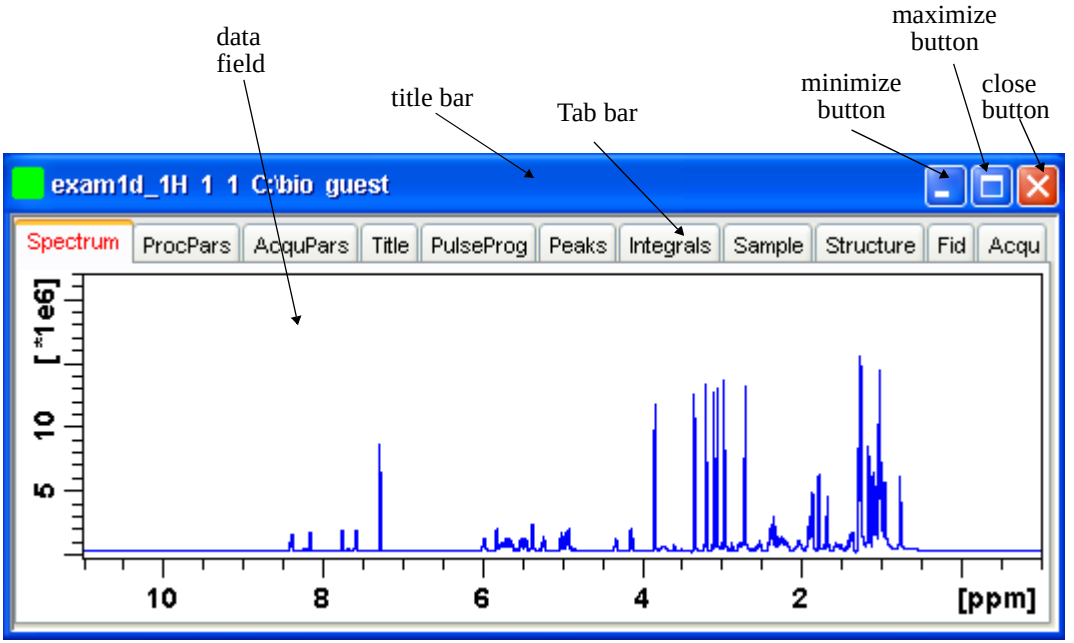


Figure 8.1

8.2 Displaying one Dataset in Multiple windows

TOPSPIN allows you to display one dataset in multiple data windows. This is, for example, convenient to view various regions or various objects (spectrum, fid, parameters etc.) of the same dataset.

How to Reopen a Dataset in a Second/Third etc. Window

1. Select (activate) the desired dataset.
2. Click ***File*** → ***Reopen*** [**`reopen`**].

Multiple data windows with the same dataset are indicated with a number in square brackets, e.g. [1], in the title bar (see Fig. 8.2).

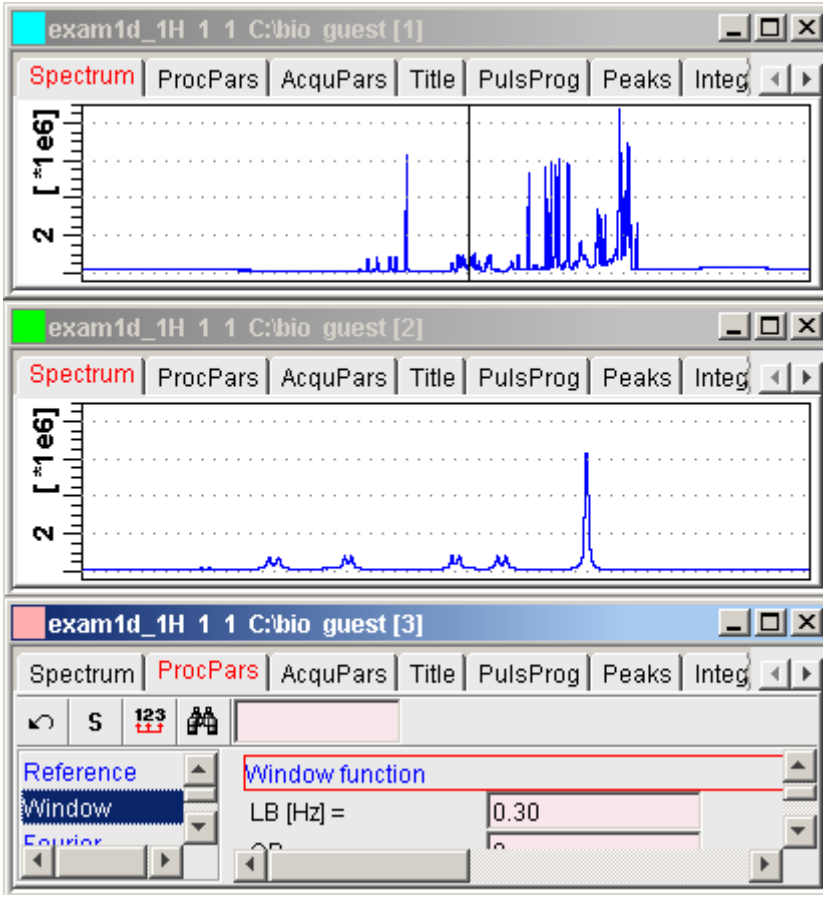


Figure 8.2

How to Rescale or Shift one Dataset in Multiple windows

Display buttons like *2 and ⤒ only work on the active data window. The same counts for the keys ***Alt***+***PageUP*** and ***Alt***+***PageDown***. However, when used with the control key, they work on all windows, for example:

☞ Hit ***Ctrl***+ *2 , ***Ctrl***+***Alt***+***PageUp*** or ***Ctrl***+***Alt***+***PageDown***

8.3 Changing the Display of a 1D Spectrum or FID

TOPSPIN offers buttons to scale or shift the spectrum vertically and horizontally.

How to Change the Vertical Scaling of the FID or Spectrum

☞ Hit one of the following the keys:

- ***Alt***+***PageUp*** : Increase the intensity by a factor of 2.
- ***Alt***+***PageDown*** : Decrease the intensity by a factor of 2.
- ***Alt***+***Enter*** : Reset the intensity.

or

☞ Click one of the following buttons:

*2 Increase the intensity by a factor of 2 [****2***].

*8 Increase the intensity by a factor of 8 [****8***].

/2 Decrease the intensity by a factor of 2 [***/2***].

/8 Decrease the intensity by a factor of 8 [***/8***].

Reset the intensity [***.vr***].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

To manipulate all data windows, press the ***Ctrl*** key while clicking one of the above buttons.

How to Smoothly Change the Vertical Scaling of the FID/Spectrum

☞ Click-hold the button and move the mouse

or

☞ Turn the mouse wheel while the cursor is in the data window.

How to Change the Horizontal Scaling of the FID or Spectrum

☞ Click-hold the button and move the mouse:

Zoom in/out smoothly.

or

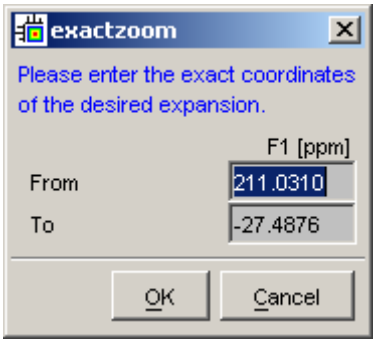
☞ Click one of the following buttons:

Zoom in to the center (spectrum) or left edge (FID) of the displayed region, increasing the horizontal scaling. [***.zi***]

Zoom out from the center (spectrum) or left edge (FID) of the displayed region, decreasing horizontal scaling) [***.zo***]

Perform an exact zoom via a dialog box [***.zx***].

a) Enter the coordinates of the desired region in the dialog box:



b) Click ***OK***

Undo last zoom [***.zl***].

Reset horizontal scaling to show the full spectrum [***.hr***].

Display the entire spectrum (baseline position and intensity scaling are adjusted if necessary) [***.all***]

Toggle interactive zoom mode. When switched off, interactive zooming only selects a horizontal region; baseline position and intensity scaling remain the same. When switched on, interactive zooming draws a box selecting the corresponding area.

Retain horizontal and vertical scaling when modifying dataset or changing to different dataset [***.keep***]. Effects all data windows.

Alternatively, you can enter the corresponding commands as specified between

square brackets [].

How to Shift a Spectral Region to the Left or to the Right

☞ Click-hold the following button and move the mouse:

 Smoothly shift to left or right.

or

☞ Click one of the following buttons:

 Shift to the left, half of the displayed region [***.sl***].

 Shift to the right, half of the displayed region [***.sr***].

 Shift to the extreme left edge of the spectrum [***.sl0***].

 Shift to the extreme right edge of the spectrum [***.sr0***].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

How to Shift the Spectrum Up or Down

To shift the FID or spectrum display up or down:

☞ Click-hold the button and move the mouse:

 Smoothly shift the spectrum baseline up/down.

or

☞ Click one of the following buttons:

 Shift the spectrum baseline to the middle of the data field [***.su***].

 Shift the spectrum baseline to the bottom of the data field [***.sd***].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

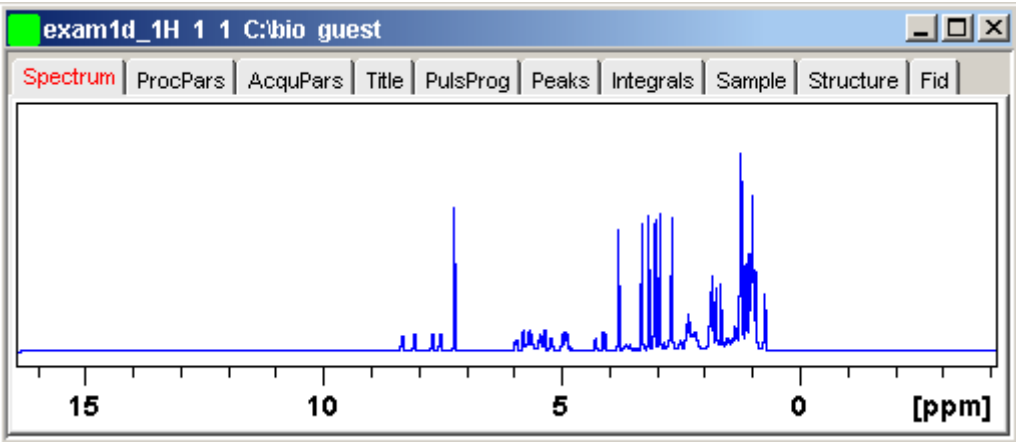
8.4 Using the Tab bar

Tabs of the data window can be activated by clicking them or by entering the corresponding commands, as specified between square brackets, on the command line. Note that command line commands always work on the currently selected (active) data window.

The Tab bar can be configured from the User Preference box (command ***set***).

How to Display the Spectrum

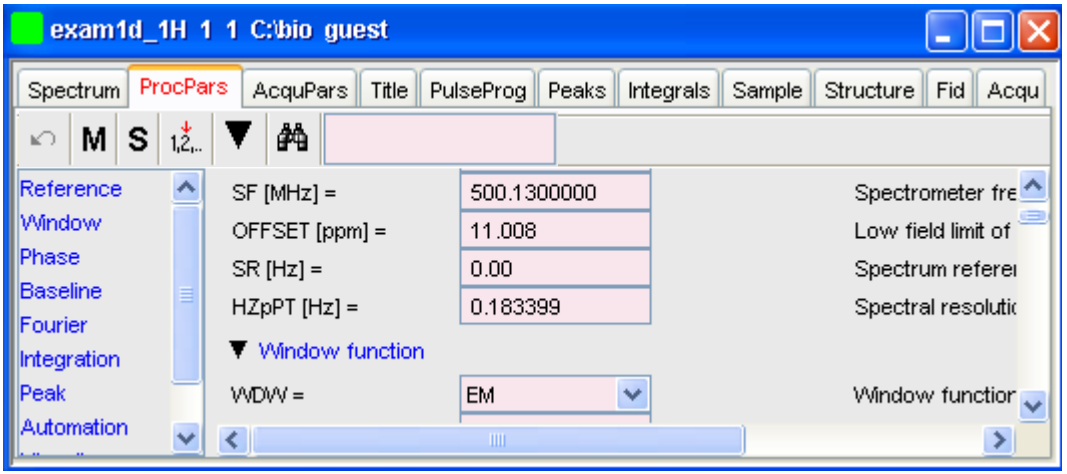
☞ Click the ***Spectrum*** tab [***spec***]



This displays the processed data. If these do not exist, the text '*No processed data available*' appears.

How to Set Processing Parameters

☞ Click the ***ProcPars*** tab [***edp***]



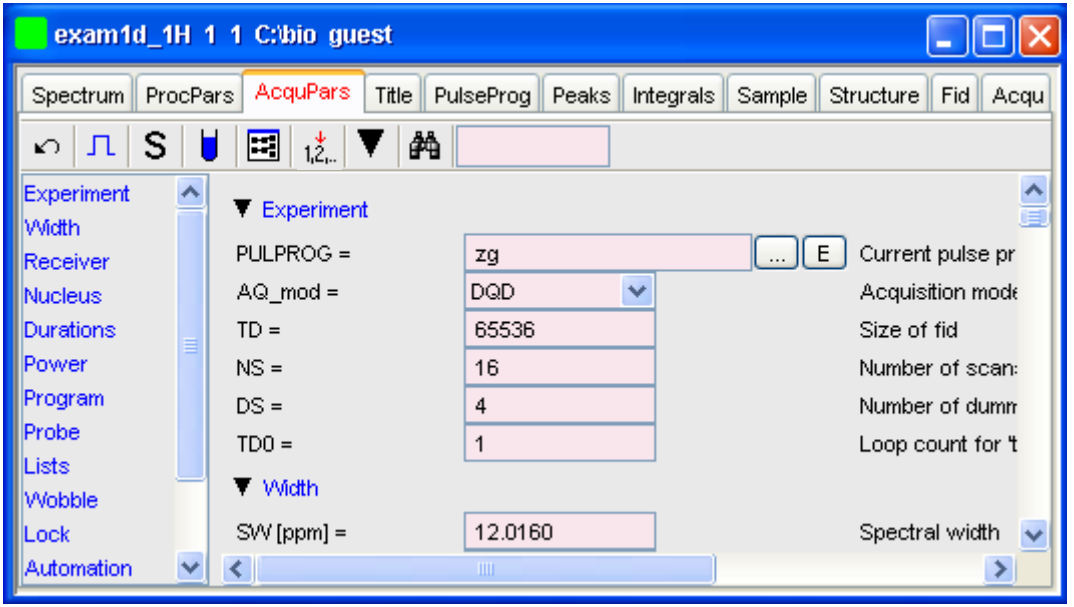
This opens the processing parameter editor (see also chapter 5.1). The following extra buttons are available:

- Undo last value change. Can be used to undo multiple changes.
- S Status parameter display. The button turns green when activated [***dpp***].
- Change processed dataset dimensionality (parameter PPARMOD).
- Collapse/expand all parameter sections.
- Search for specified parameter.

Changed parameters are automatically saved.

How to Set Acquisition Parameters

☞ Click the ***AcquPars*** tab [**eda**]



This opens the acquisition parameter editor (see also chapter 5.1)). The following extra buttons are available:

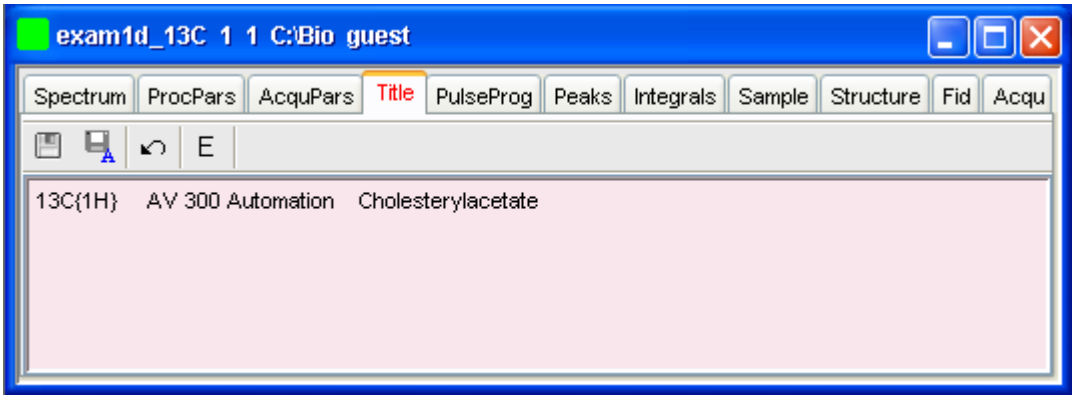
- Undo last value change. Can be used to undo multiple changes.
- Show pulse program parameters [**ased**].
- Status parameter display. The button turns green when activated [**dpa**].
- Set probehead/solvent dependant parameters [**getprosol**].
- Set nuclei and routing [**edasp**]
- Change raw dataset dimensionality (parameter PARMODE).
- Collapse/expand all parameter sections.
- Search for specified parameter.

Changed parameters are automatically saved.

Note that the **...** and ***E*** button to the right of the PULPROG parameter allow you to show the pulse program list or edit the current pulse program, respectively.

How to Edit the Title

Click the ***Title*** tab [**`edti`**]



This allows you to edit the title that appears in the data window and on the plot.

- Save the title file under its current name.
- Save the title file under a new name.
- Reload the title file. Undo modifications since the last save.
- E Open the title file with the external editor (defined in User Preferences).

How to Edit the Pulse Program

☞ Click the ***PulsProg*** tab [***edcpul***]



This allows you to edit the current pulse program. The following extra buttons are available here:

- Save the pulse program under its current name.
- Save the pulse program under a new name.
- Reload the pulse program. Undo modifications since the last save.
- Switch to status pulse program.
- Show the pulse program in an external editor.
- Start the graphical pulse program display [***nmrsim***].
- Search in the pulse program.
- Search for more info in the knowledge base

How to Display the Peak list

Click the ***Peaks*** tab



Peak	Index (F1)	v(F1) [ppm]	Intensity [abs]	Intensity [rel]	Half width [ppm]
1	19569.9	3.8319	11472303.78	11.04	0.0044
2	20929.9	3.3332	12495443.09	11.95	0.0037
3	**21320.4**	**3.1900**	**13371661.03**	**12.67**	**0.0037**
4	21603.7	3.0861	12663022.38	12.03	0.0040
5	21707.1	3.0482	13159654.59	12.36	0.0037
6	**21947.3**	**2.9601**	**13733719.44**	**12.93**	**0.0033**
7	22658.2	2.6994	13251895.75	12.48	0.0040
8	26579.7	1.2614	15909845.88	15.00	0.0059
9	26615.4	1.2483	13804594.47	12.98	0.0077

Figure 8.3

This displays the peak list. By default, the peak list shows the following entries:

Peak : the peak number

v(F1) [ppm] : the chemical shift

Intensity [abs]: the absolute peak intensity

Intensity [rel]: the relative peak intensity

Half width [ppm]: the peak width at half-height

Display the spectral region around a peak

☞ Right-click the desired peak

this will open the popup menu shown in Fig. 8.4.

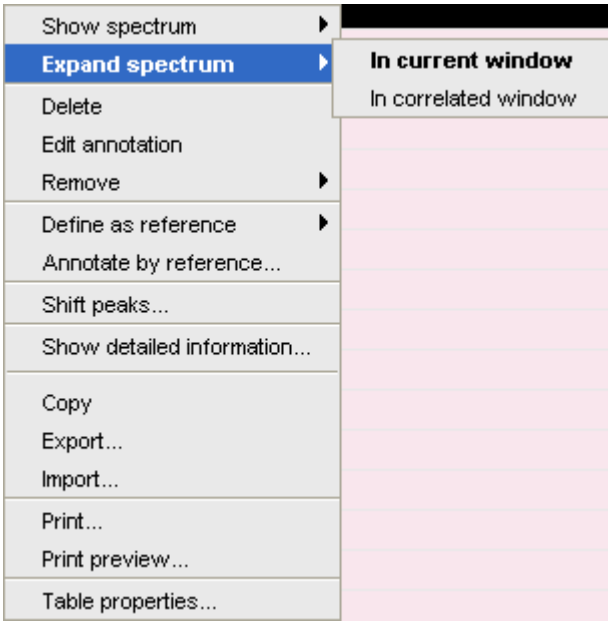


Figure 8.4

Here you can choose from the following options:

☞ ***Show spectrum → In correlated window***
to open a new data window showing the full correlated spectrum

☞ ***Expand spectrum → In current window***
to change the current data window to spectrum display, showing the region around the selected peak

☞ ***Expand spectrum → In correlated window***
to open a new data window showing the region around the selected peak

☞ ***Edit Annotation***
Edit the annotation of the current integral.

☞ ***Define as reference → Complete table***
Define the entire peak table as a reference for annotation.

☞ ***Define as reference → Selection***
Define the selected peaks as a reference for annotation.

☞ ***Annotate by reference...***
Create annotations according to the peaklist of the reference dataset. You will be prompted for the allowed variation in chemical shift.

☞ ***Shift peaks...***
Shift all peaks. You will be prompted for the number of ppm to be shifted.

☞ ***Show detailed information***
Show peak information, dataset information and peak picking parameters.

Export entries of the peak list

Entries of the peak list can easily be exported to Excel or any other program as follows:

1. For multiple peaks:

   Select the desired entries while pressing the ***Ctrl*** or ***Shift*** key
2. Right-click a peak entry to open the popup menu (see Fig. 8.4).
3. Click ***Export...*** to export the selected peaks.
4. This opens a dialog box where you can specify the filename and file type. For the latter you can choose from:
   - Auremol peaklist (.ml)
   - Comma Separated Values (.cvs)
   - Mixed Shape deconvolution peak list (.peaklist)
   - TOPSPIN peak list (.xml)
   - XEASY peak list (.peaks)
   - XWIN-NMR peak list (.txt)

   Important: Check the box in the lower-left corner to export the selected peaks only or uncheck it to export the entire list. Then click ***Export***.

Delete/remove peaks from the peak list

To delete one peak:

☞ Right-click the peak and choose ***Delete*** from the popup menu

To delete multiple peaks:

1. Select the peaks while pressing the ***Ctrl*** or ***Shift*** key
2. Right-click one of the peaks and choose ***Delete*** from the popup menu

To remove possible duplicate peaks:

☞ Right-click any entry and choose ***Remove*** → ***Duplicate peaks***

To remove possible peaks outside of the spectrum:

☞ Right-click any entry and choose ***Remove*** → ***Peaks positioned outside of the spectrum***

To remove solvent peaks:

☞ Right-click any entry and choose ***Remove*** → ***Solvent Peaks***

Copy the peak List

Instead of exporting entries of the peak list, they can also be copied to the Clipboard and pasted to another application like Excel. To do that:

1. For multiple peaks:

   Select the desired entries while pressing the ***Ctrl*** or ***Shift*** key
2. Right-click a peak entry to open the popup menu (see Fig. 8.4).
3. Click ***Copy...*** to copy the selected peaks to the Clipboard.

Print the peak List

To print the peaklist:

☞ Right-click a peak entry and choose ***Print...***

or

☞ Enter ***print*** on the command line

or

☞ Press ***Ctrl-p***

☞ All actions will print the entire peaklist.

To preview a print:

☞ Right-click a peak entry and choose ***Print preview...***

☞

Import a peak List

A peak list from a different dataset or program can be imported as follows:

1. Right-click an entry to open the popup menu (see Fig. 8.4).
2. Click **Import...**
3. In the appearing dialog box, navigate to the directory where the list resides and select the peak list, choosing from:
   - Auremol peaklist (.ml)
   - MULABEL peak list (labels)
   - TOPSPIN peak list (.xml)
   - XEASY peak list (.peaks)
   - XWIN-NMR peak list (.txt)

As such you can import a peak list from a different dataset or program or a previously exported list from the current dataset. Note that peak picking commands store the peak list in the processed data directory under the name `peak.xml` (TOPSPIN 2.1 or newer) or `peak.txt` (XWIN-NMR and TOPSPIN 2.0 or older).

Shortcuts

Double-click a peak : zoom into spectrum, i.e. show region around that peak.

Enter key : zoom into spectrum, i.e. show region around selected peak(s).

Delete key : delete the selected peak(s) from the peak list.

Ctrl+***c*** : copy selected peaks to the Clipboard.

Ctrl+***a*** : select all peaks.

Home : select the first peak.

End : select the last peak.

Shift+***Home*** : select current and first peak and all in between.

Shift+***End*** : select current and last peak and all in between.

Note that these keys only work when the cursor focus is in the data window.

Table properties:

Various properties of the peak table can be configured. To do that:

1. Right-click an entry to open the popup menu (see Fig. 8.4).
2. Click **Table properties...**

3. In the appearing dialog box, with 3 tabs:

- ***Columns***
  Allows you to select the columns to be displayed, set the column width and the number of fraction digits. Furthermore, you can switch on/off scientific notation of values for each column individually.
- ***Colours***
  Allows you to set various colours of the table.
- ***Spacings***
  Allows you to set various spacings of the table

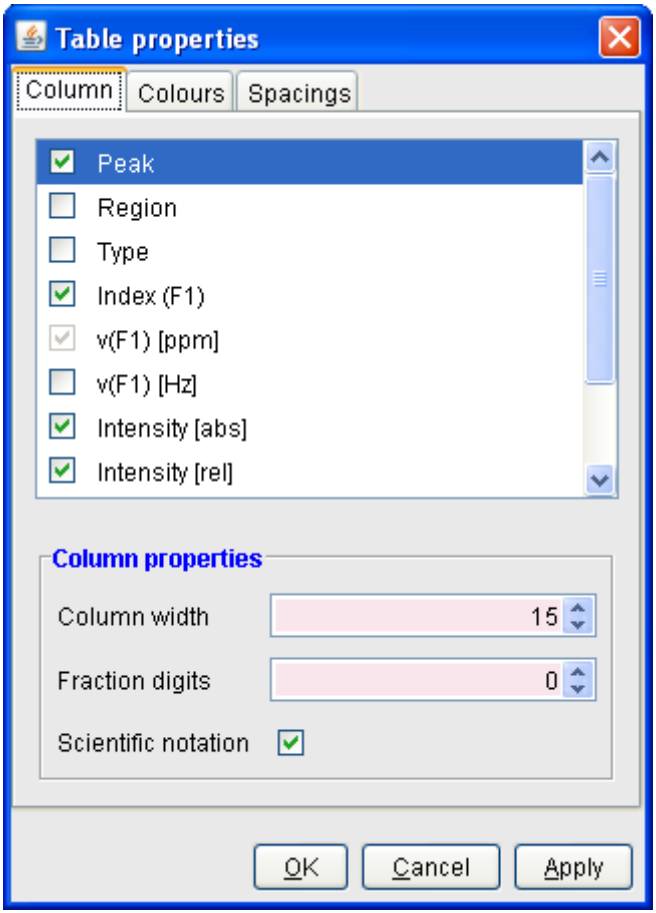


Figure 8.5

When you move the cursor over the peak list, the active peak will, by default, be highlighted in blue (see peak 3 in Fig. 8.6). If the correlated spectrum is also displayed, a vertical line moves along, showing corresponding position in the spectrum (see Fig. 8.6)

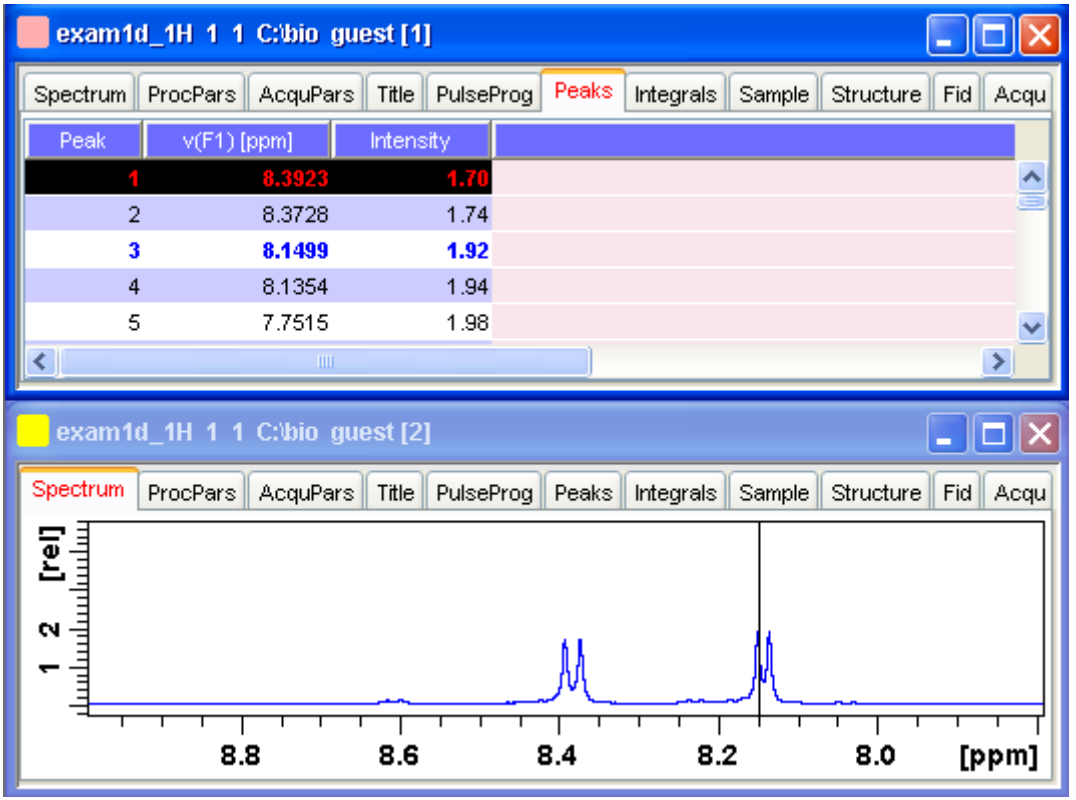

exam1d_1H 1 1 C:\bio guest [1]
Spectrum ProcPars AcquPars Title PulseProg Peaks Integrals Sample Structure Fid Acqu
Peak v(F1) [ppm] Intensity
1 8.3923 1.70
2 8.3728 1.74
3 8.1499 1.92
4 8.1354 1.94
5 7.7515 1.98
exam1d_1H 1 1 C:\bio guest [2]
Spectrum ProcPars AcquPars Title PulseProg Peaks Integrals Sample Structure Fid Acqu
1 2 [rel]
8.8 8.6 8.4 8.2 8.0 [ppm]

Figure 8.6

As soon as you click a peak, it is selected and, by default, displayed in red (see peak 1 in Fig. 8.6). Note that this peak remains selected, i.e. is used by ***Enter*** and ***Delete***, until a different peak is selected.

To extend the peak list with *Regions*, *Type* and *Index* entries, right-click any part of the header bar.

To sort the peaks according to peak number, ppm value or intensity, click the header of the respective entry.

Note that when you delete peaks from the peak list, they are automatically removed from the corresponding file. You cannot undo a delete action.

Peaks are only available if peak picking has been done (command ***pp***). The peak list can be printed with ***print*** [***Ctrl***+***p***]. List items can be selected with the

mouse, copied with ***Ctrl*+*c*** and pasted to other applications, e.g. a text editor.

How to Display the Integral list

☞ Click the ***Integrals*** tab **[*li*, *lipp*, *lippf*]**

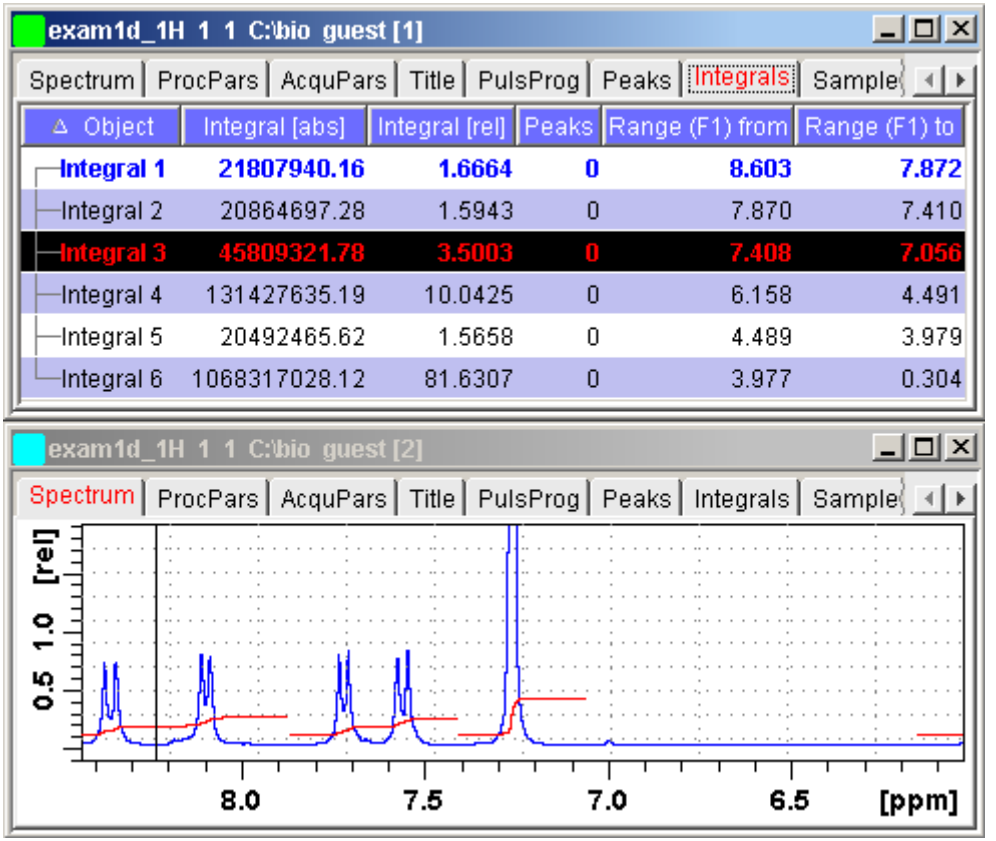


Figure 8.7

This displays the integral list (upper part of Fig. 8.7). By default, this shows the following items:

Object : the integral number

Integral [abs] : the absolute integral value

Integral [rel] : the relative integral value

Peaks : the number of peaks within the integral range

Range (F1) from : the left edge of the integral range

Range (F1) to : the right edge of the integral range

Please note the difference between the following items:

- **selected integral**: the entry that has been clicked last (Integral 3 in Fig. 8.7). If you right-click an entry, it is selected and you can execute one of the commands from the popup menu (see Fig. 8.8) The keys **`Enter`** and **`Delete`** work on the selected entry.
- **active integral**: the entry on which cursor resides (Integral 1 in Fig. 8.7). The active integral is also marked in the correlated spectrum by a black vertical line (see lower part of Fig. 8.7 and description below). When you move the cursor over the integral list, the vertical line in the correlated spectrum moves along with it and vice versa.

Note that the colours of the selected and active integral can be set in the table properties (see above).

Display the spectral region around an integral

To display the spectral region around a particular integral:

☞ Right-click the desired integral

This will open the popup menu shown in Fig. 8.8.

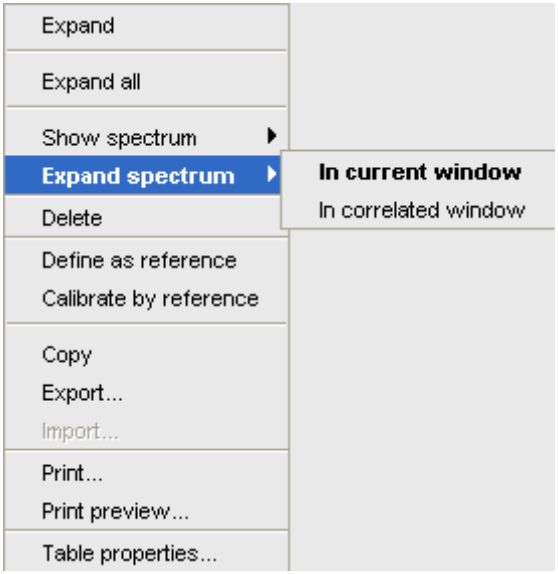


Figure 8.8

Here you can choose from the following options:

- ☞ ***Show spectrum → In correlated spectrum***
  to open a new data window showing the full correlated spectrum
- ☞ ***Expand spectrum → In current window***
  to change the current data window to spectrum display, showing the region around the selected integral
- ☞ ***Expand spectrum → In correlated window***
  to open a new data window showing the region around the selected integral (lower part of Fig. 8.7)

Note that clicking the marked entry in the right-click popup menu is equivalent to pressing of the ***Enter*** key.

Export/Import Entries of the Integral List

Entries of the integral list can easily be exported to Excel or any other program as follows:

1. For multiple integrals:

Select the desired entries while pressing the ***Ctrl*** or ***Shift*** key

2. Right-click an entry to open the popup menu (see Fig. 8.8)
3. Click one of the following menu items:
   - ***Copy***
     Copy the selected integral(s) entry to the Clipboard. Equivalent to clicking ***Edit*** → ***Copy*** or hitting ***Ctrl+c***. Copied integrals can easily be pasted in any other application such as Excel.
   - **Export...**
     Export selected integrals. Check the box in the lower-left corner to export the selected integrals only or uncheck it to export the entire list. Then click ***Export***.

Calibrate Integrals to Compare Spectra

Integrals from the current and other spectra can be calibrated with respect to a reference integral. To do that:

1. Right-click the reference integral and choose **Define as reference** from the popup menu. This will determine the calibration constant.
2. Right-click any integral and choose ***Calibrate by reference***
   This will divide all integrals by the calibration constant, setting the reference integral to 1.0.

Now you can read any other spectrum, and calibrate its integrals with respect to the reference integral defined above. To do that:

1. Read the spectrum
2. Enter ***int*** to define the integral ranges (if this has not been done yet)
3. Click the ***Integrals*** tab
4. Right-click any integral in the list and choose ***Calibrate by reference*** from the popup menu.

Note that the calibration constant is lost when TOPSPIN is restarted.

Display the integral list with peaks

The integral list in Fig. 8.7 shows only integrals. However, if peak picking has been done, the integral list also shows the peaks within each integral range (see Fig. 8.9).

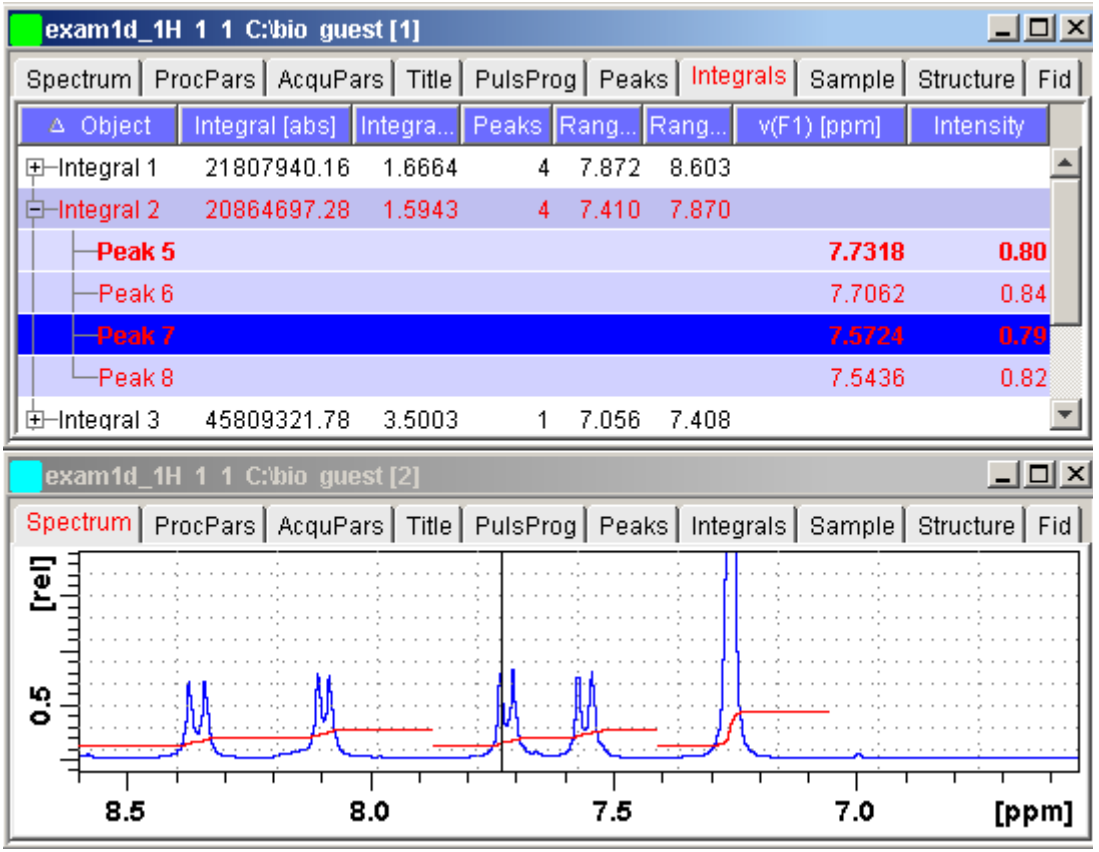


Figure 8.9

Note that the integral entries can be collapsed, (hiding the peaks) or expanded (showing the peaks). As soon as one or more integrals entries are expanded, two extra columns appear showing:

v(F1) [ppm] : the chemical shift of the peak

Intensity: the peak intensity

Depending on whether or not integrals are expanded, the right-click popup menu contains the following extra items:

- ***Expand***
  Expand the current integral showing all peaks within it.

- ***Expand all***
  Expand all integrals showing all peaks within them.
- ***Collapse all***
  Collapse all integrals hiding all peaks within them.

In addition to the integral entry, an individual peak within an integral can be activated (by placing the cursor on it) or selected (by clicking it). In Fig. 8.9, peak 7 is selected and the correlated spectrum is displayed. Peak 5 is active which is also shown by the vertical line in the correlated spectrum.

Delete an Integral from the Integral List

To delete one integral:

☞ Right-click the integral and choose ***Delete*** from the popup menu

To delete multiple integrals:

1. Select the integrals while pressing the ***`Ctrl`*** or ***`Shift`*** key
2. Right-click one of the integrals and choose ***Delete*** from the popup menu

Note that these keys only work when the cursor focus is in the data window.

Table properties:

Various properties of the integral table can be configured. To do that:

1. Right-click an entry to open the popup menu (see Fig. 8.10).
2. Click **Table properties...**
3. In the appearing dialog box, with 3 tabs:
4. ***Columns***
   Allows you to select the columns to be displayed, set the column
   - width and the number of fraction digits. Furthermore, you can switch on/off scientific notation of values for each individual column.
   - ***Colours***
     Allows you to set various colours of the table.
   - ***Spacings***
     Allows you to set various spacings of the table

5.

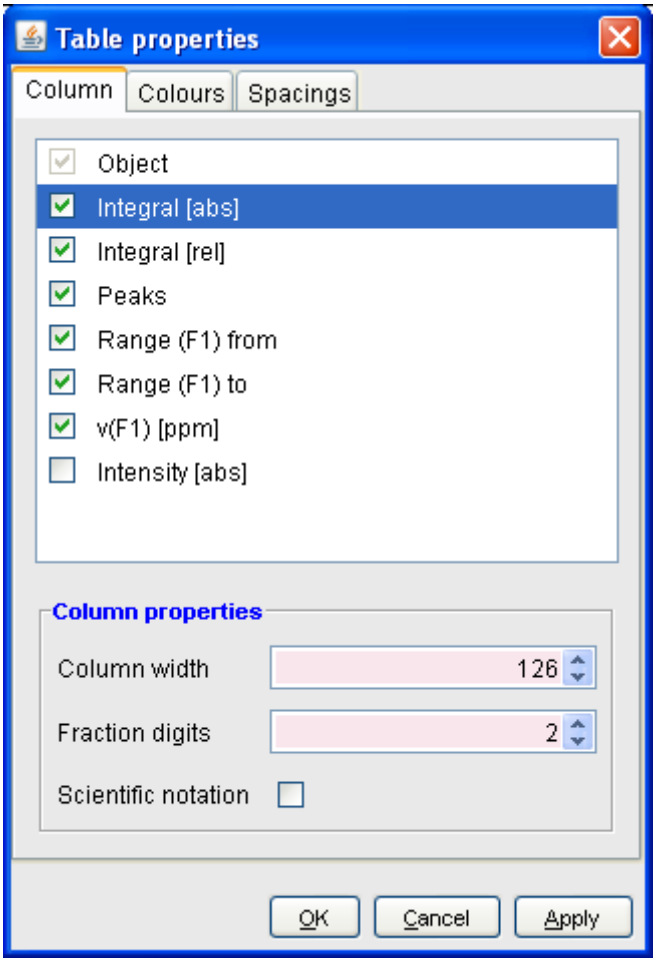


Figure 8.10

Shortcuts

Enter key : zoom into spectrum, i.e. show region around selected integral(s))

Delete key : delete the selected integral(s) from the integral list

Ctrl+c : copy selected integrals to the Clipboard.

Ctrl*+*a : select all peaks.

Home : select the first peak

End : select the last peak

Shift*+*Home : select current and first peak and all in between

Shift*+*End : select current and last peak and all in between

Double-clicking an integral will show the peaks within the integral region if they exist. It they do not exist, it will zoom into spectrum showing the integral region.

Note that these keys only work when the cursor focus is in the data window.

How to view Sample Information

☞ Click the ***Sample*** tab [***edsam***]

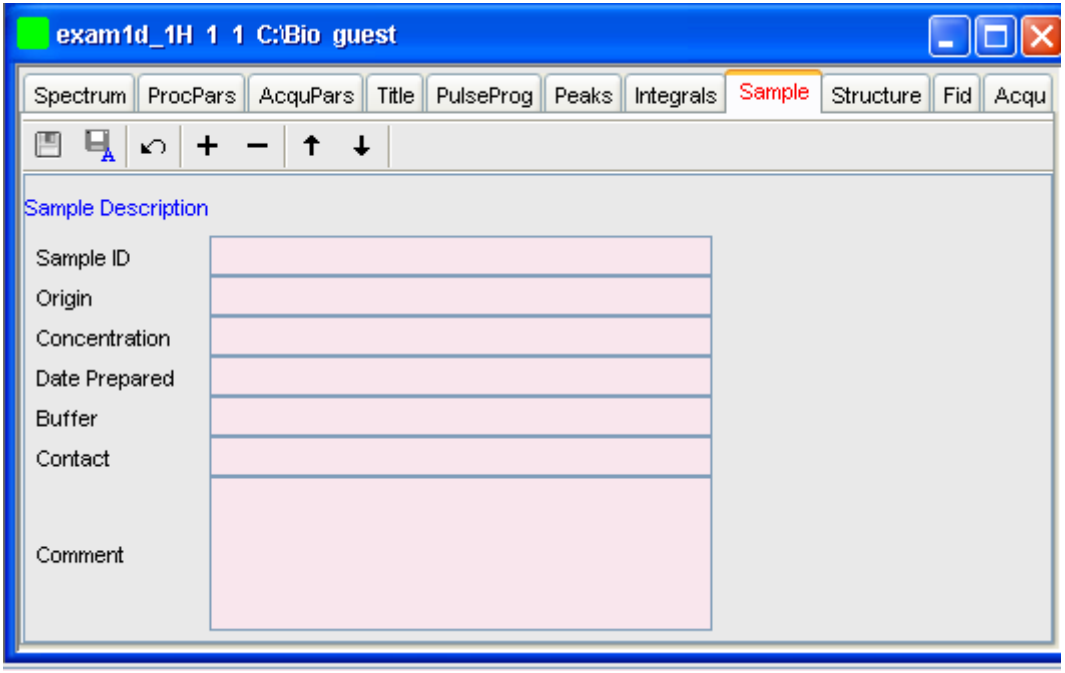


Figure 8.11

This table can be used to fill out any sample information you want to store with

the dataset. The table can easily be modified or extended with the following functions:

To select an item: double-click it!

Save the sample information table with the dataset.

Save the sample information table as default.

Reload the original table discarding any changes

Add a new item to the table. You will be prompted for an identification name and the desired number of lines

Remove the selected item from the table

Move the selected item one place up in the table

Move the selected item one place down in the table

How to Open the Jmol Molecule Structure Viewer

☞ Click the ***Structure*** tab [`jmol`]:

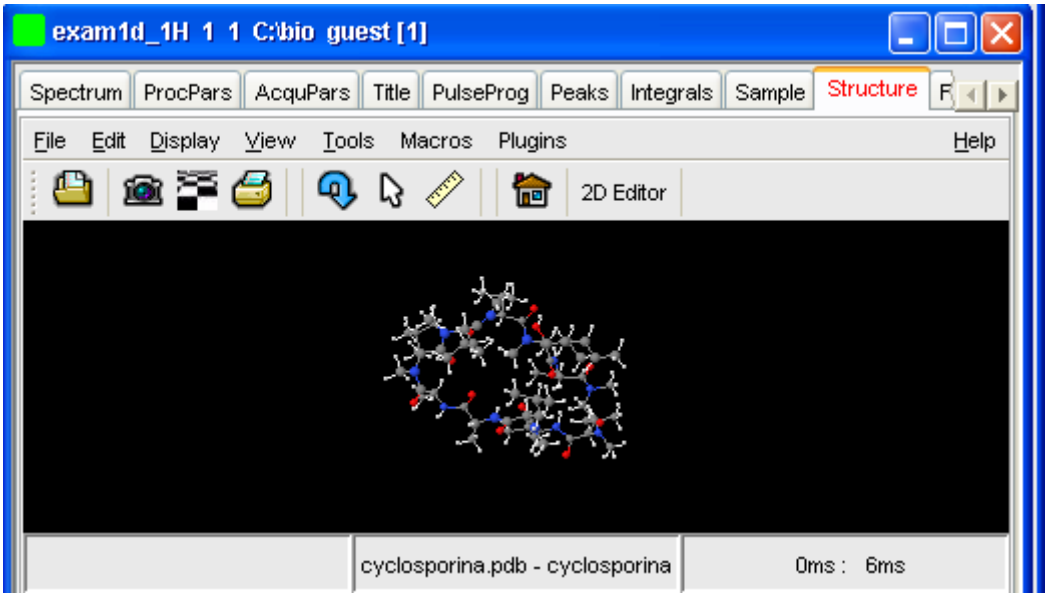


Figure 8.12

opens the *Jmol* molecule structure viewer. TOPSPIN 2.1 contains Jmol version 10. This has the following features:

- The viewer displays the structure file that resides in the *expno* of the current dataset. If this does not exist, the structure file defined by the acquisition parameter CHEMSTR is displayed. CHEMSTR can define a full pathname or a filename. In the latter case, the file is searched for in the directory defined in the User Preferences. To set this directory, click ***Options → Preferences***, select ***Directory path names***, enter a directory and click ***OK***. If no structure file is found, you can open one by clicking ***File → Open*** in the Molecule Viewer
- The following structure file types are supported: `.xyz`, `.mol`, `.pdb`, `.cml`, `.out`, `.mmlgp`, `.res`, `.cif`, `.gpr`, `.hin`, `.nwo`.
- Secondary structure elements of proteins (backbone, cartoons, ribbons, ...) can be displayed in selectable sizes and colors.
- Mouse button effects:

  Rotate a molecule around the x- and y-axis by pressing the left mouse button, and moving the mouse left/right or up/down, respectively.

  Rotate a molecule around the z-axis by pressing the middle mouse button and moving the mouse left/right .

  Zoom in or out a molecule by pressing the middle mouse button, and moving the mouse up or down.

- RASmol command scripts are supported. To send a RASmol command to the currently displayed molecule enter:

  ☞***jmol <RASmol command>***

  Here are some example:

  ☞***jmol zoom 400***

  ☞***jmol ribbon 200***

  ☞***jmol color ribbon yellow***

  You may create TOPSPIN macros containing RASmol commands. Just enter ***edmac*** on the TOPSPIN command line and insert the RASmol commands in the appearing editor. Here is an example:

  ```
  jmol load /mystructures/alphahelix.pdb # load a structure
  ```

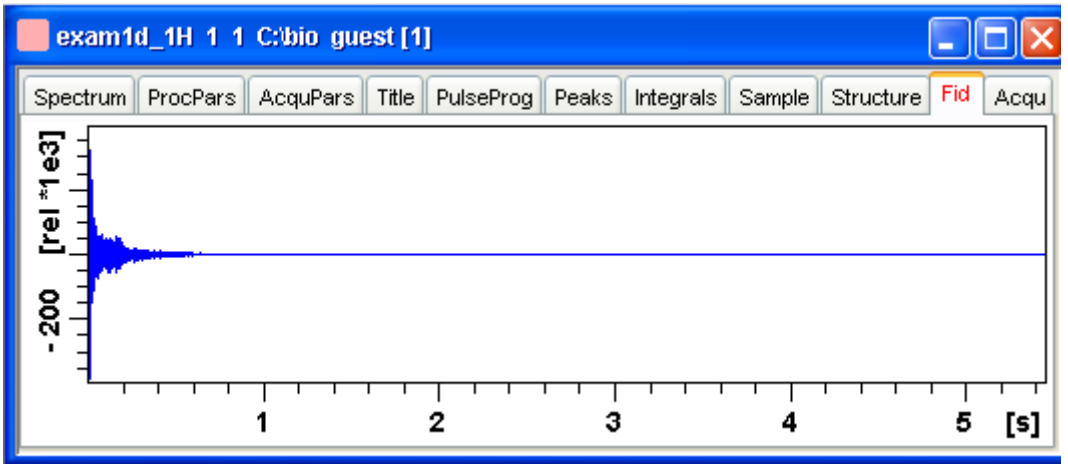
```
jmol backbone 0.7 # display its backbone with 0.7 Angstrom size
jmol color backbone yellow # change backbone color
jmol background green # change background color
jmol zoom 200 # zoom structure
```

The available RASmol commands are described in the ***Jmol*** Help menu.

- Multiple molecules (or multiple aspects of one molecule) can be displayed simultaneously. To do that just open multiple data sets or open the same dataset in multiple data windows and click on the ***Structure*** Tab in each window.

How to Display the FID

☞ Click the ***Fid*** tab [***fid***]



displays the raw data. If these do not exist, the text '*No raw data available*' appears. The following additional buttons appear at the right of the lower toolbar:

Show FID in shuffled mode

Show FID in unshuffled mode

If you open a new dataset, the ***Spectrum*** tab is activated, no matter which tab was selected before. If you enter any interactive mode, for example phase correction mode, the Tab bar is replaced by a toolbar for that mode.

8.5 1D Display Options

How to Toggle between Hertz and ppm Axis Units

Click the following toggle button in the upper toolbar:


Toggle between Hz and ppm axis units [***.hz***]

How to Switch on/off the Spectrum Overview display

The spectrum overview shows the entire spectrum at the top of the data window. It is useful when only a certain region of the spectrum is displayed. In the overview, the displayed region is marked as a green area. To switch on the spectrum overview, click the following toggle button in the upper toolbar:


Switch the spectrum overview display on/off [***.ov***]

To shift the displayed region, simply click-hold the green area in the overview spectrum and move the mouse (see Fig. 8.13).

How to Switch Y-axis Display

Click the following toggle button in the upper toolbar:


Switch the y-axis display between abs/rel/off [***.y***]

Fig. 8.13 shows a data window with the spectrum overview on, ppm axis units, and

absolute y-axis display.

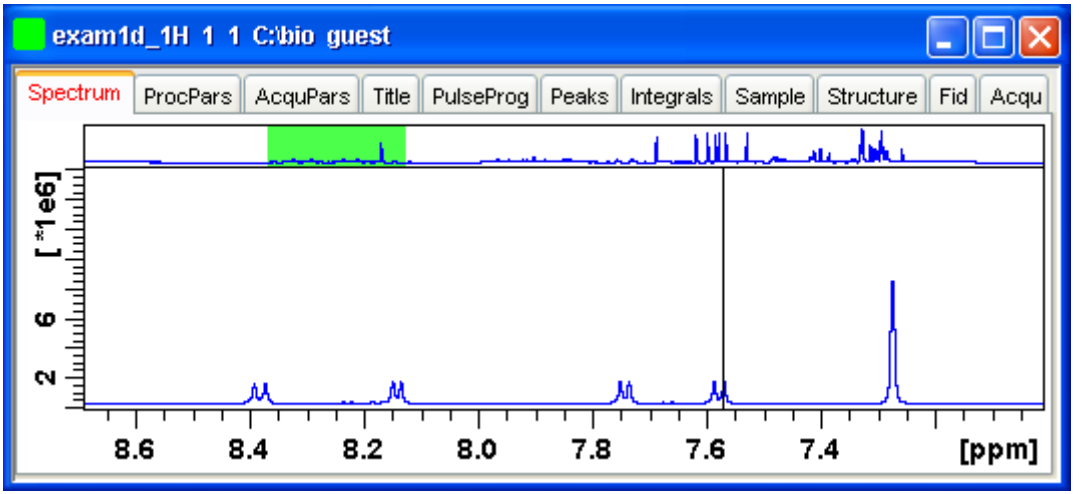


Figure 8.13

8.6 Show Display Properties/Regions/Files

If you right-click inside the data window, the following popup menu will appear:



If you choose ***Display Properties...***, a dialog box (see Fig. 8.14) will appear.

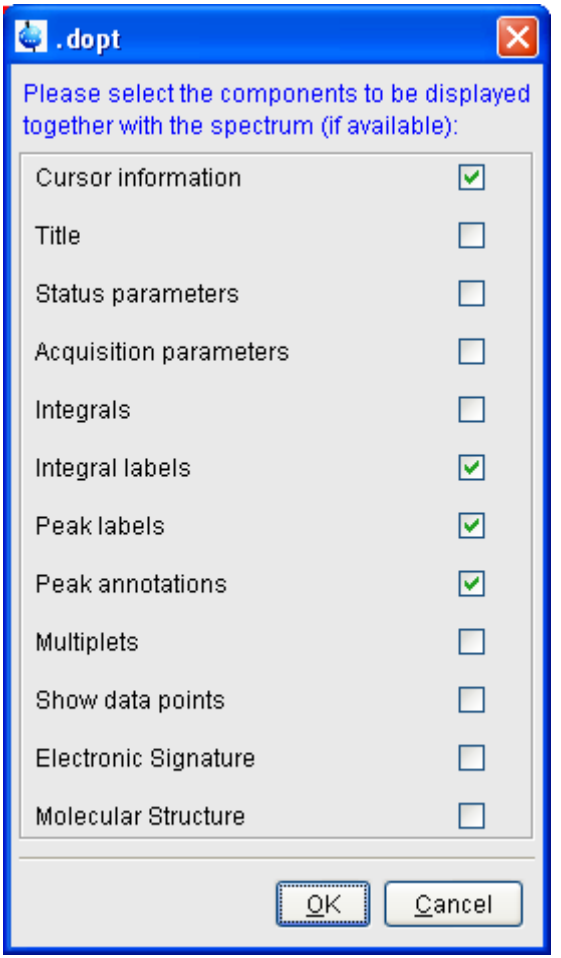


Figure 8.14

Here you can check or uncheck the spectrum components that you want to be displayed in the data window.

Note that the ***Display Properties...*** dialog box can also be opened from the ***View*** menu.

How to Superimpose the Cursor Information

To superimpose the cursor information on the spectrum:

1. Right-click in the data window and choose ***Display Properties*** [**`.dopt`**]
2. Check ***Cursor information*** in the appearing dialog box and click ***OK***

How to Superimpose the Title on the Spectrum

1. Right-click in the data window and choose ***Display Properties...*** [**`.dopt`**]
2. Check ***Title*** in the appearing dialog box and click ***OK***

How to Superimpose the main Status Parameters on the Spectrum [1]

1. Right-click in the data window and choose ***Display Properties...*** [**`.dopt`**]
2. Check ***Status parameters*** in the appearing dialog box and click ***OK***

How to Superimpose the Integral Trails/Labels on the Spectrum

1. Right-click in the data window and choose ***Display Properties...*** [**`.dopt`**]
2. Check ***Integrals*** and, if desired, ***Integral labels*** in the appearing dialog box
3. Click ***OK***

If no integrals appear, the integral regions have not been determined yet. This can be done with the **`int`** command.

How to Superimpose Peak Labels on the Spectrum

1. Right-click in the data window and choose ***Display Properties...*** [**`.dopt`**]
2. Check ***Peak labels*** in the appearing dialog box and click ***OK***

If no peak labels appear, peak picking has not been done yet. This can be done with the **`pp`** command.

How to Show Peak Annotations on the Spectrum

1. Right-click in the data window and choose ***Display Properties...*** [**`.dopt`**]
2. Check ***Peak labels*** and ***Peak Annotations*** in the appearing dialog box and click ***OK***

Peak annotations appear, on peaks for which annotations have been defined, instead of regular peak labels showing chemical shift values. If no peak labels or annotations appear, peak picking has not been done yet. This can be done with the

1. These are the status parameters that also appear on the plot.

pp command.

How to Show Individual Data Points of the Spectrum

1. Right-click in the data window and choose ***Display Properties...*** [***.dopt***]
2. Check ***Show data points*** in the appearing dialog box and click ***OK***
3. Expand the spectral region where you want to see individual points.

How to Superimpose the Electronic Signature on the Spectrum

1. Right-click in the data window and choose ***Display Properties...*** [***.dopt***]
2. Check ***Electronic Signature*** in the appearing dialog box and click ***OK***

The electronic signature, entered with ***esign***, will appear below the title.

How to Display the Main Dataset Properties

☞ Right-click inside the data window and choose ***File Properties***

An information box as displayed in Fig. 8.15 will appear.

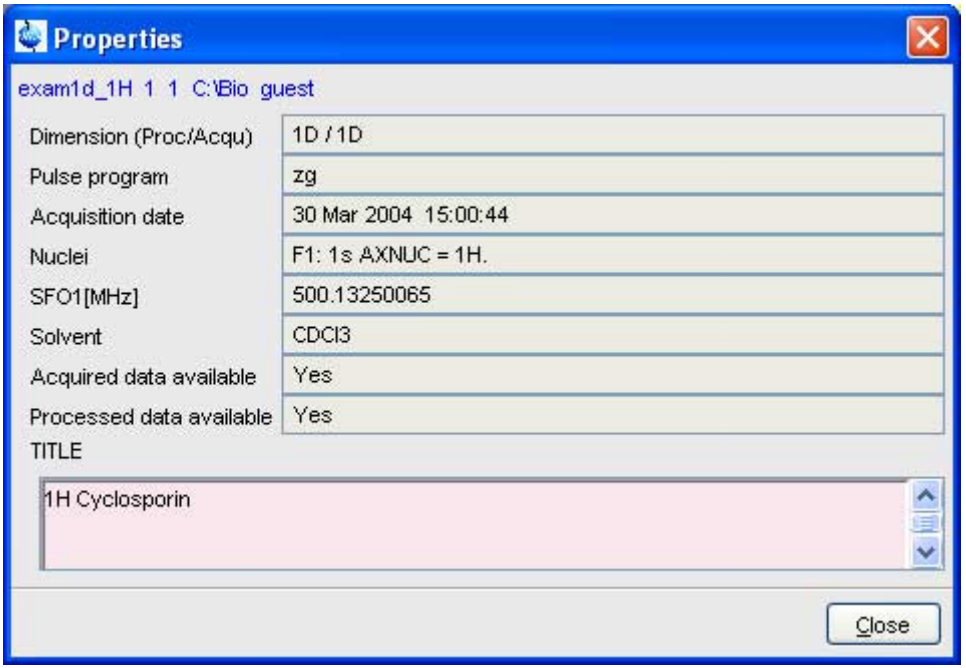


Figure 8.15

Note that this is status information which cannot be changed.

How to Display a List of Files of a Dataset

☞ Right-click inside the data window choose ***Files***

Fig. 8.16 shows the file list when the ***Fid*** tab is active, i.e. when the raw data are displayed. It is the contents of the *expno* directory.

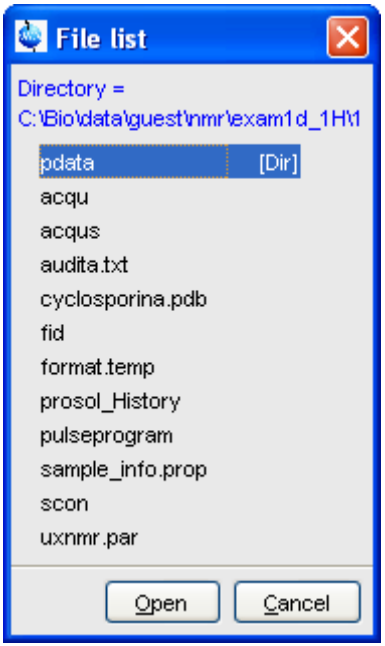


Figure 8.16

Fig. 8.17 shows the file list that appears when the ***Spectrum*** tab is active, i.e. when the processed data are displayed. It is the contents of the *procno* directory.

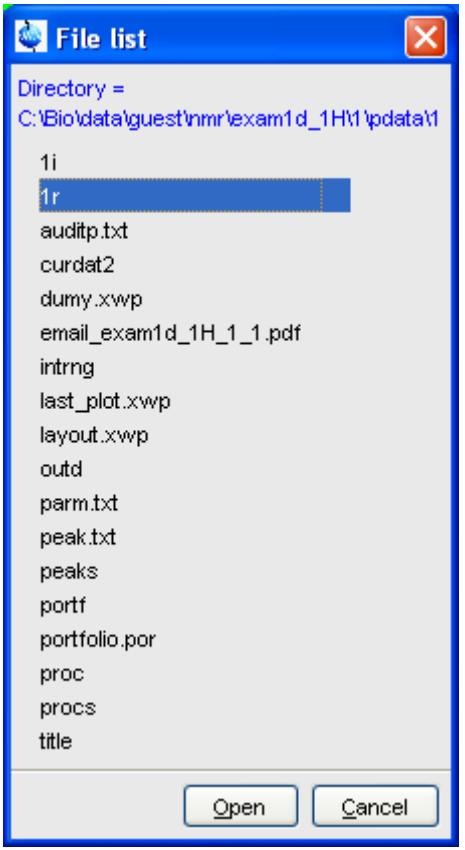


Figure 8.17

The contents of any file in the list can be displayed as follows:

1. Select a filename (it will be highlighted)
2. Click ***Open***

Note that this only makes sense for ascii files, e.g. `acqu*`, `proc*` or files with the extension `.txt`.

Dataset files can also be displayed/opened with the command ***`expl`***. This opens the Windows Explorer, or under Linux, the Konqueror or Mozilla, showing the contents of the *procno* directory.

8.7 Saving Display Region

The currently displayed spectral region can be stored as follows:

☞ Right-click in the data window and choose ***Save Display Region To...***

This will open the dialog box shown in Fig. 8.18.

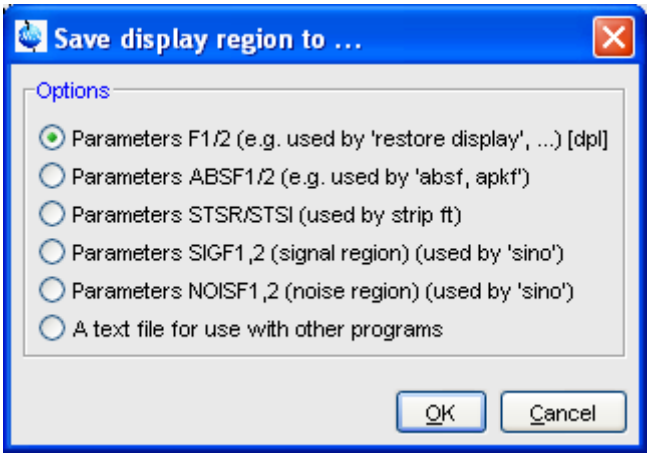

Save display region to ...
Options
Parameters F1/2 (e.g. used by 'restore display', ...) [dpl]
Parameters ABSF1/2 (e.g. used by 'absf, apkf')
Parameters STSR/STSI (used by strip ft)
Parameters SIGF1,2 (signal region) (used by 'sino')
Parameters NOISF1,2 (noise region) (used by 'sino')
A text file for use with other programs
OK
Cancel

Figure 8.18

Here the following options are available:

- **Parameters F1/2** [***dpl***]

  to save the displayed region for restoring the display later. The region is stored in the parameters F1P and F2P.

To restore the saved region, right-click in the data window and choose:

Restore Display Region from Params F1/2

- **Parameters ABSF1/2**

  to save the displayed region for baseline correction (command ***absf***) or phase correction (command ***apkf***). The region is stored in the processing parameters ABSF1 and ABSF2.

- **Parameters STSR/STSI**

  to save the displayed region for Strip FT (commands like ***ft*** and ***trf***). The

region is stored in the processing parameters STSR and STSI.

- **Parameters NOISF1/2**

  to save the displayed region as the signal region for Signal to Noise calculation (command ***sino***). The region is stored in the processing parameters SIGF1 and SIGF2.

- **Parameters SIGF1/2**

  to save the displayed region as the noise region for Signal to Noise calculation (command ***sino***). The region is stored in the processing parameters NOISF1 and NOISF2.

- **A text file for use with other programs**

  to save the displayed region in a text file. This file can be viewed with any editor or used by external programs.

8.8 Synchronize Visible Region of all Data Windows

The visible region of all data windows can be synchronizes as follows.

☞ Zoom in or out one dataset while holding the ***Ctrl*** key

or

☞ Zoom in or out one dataset and then enter the ***.sync*** command

Chapter 9

2D Display

9.1 The 2D Data Window

The 2D data window consists of a data field, a title bar, a Tab bar and buttons. Fig. 9.1 shows a data window with a 2D spectrum.

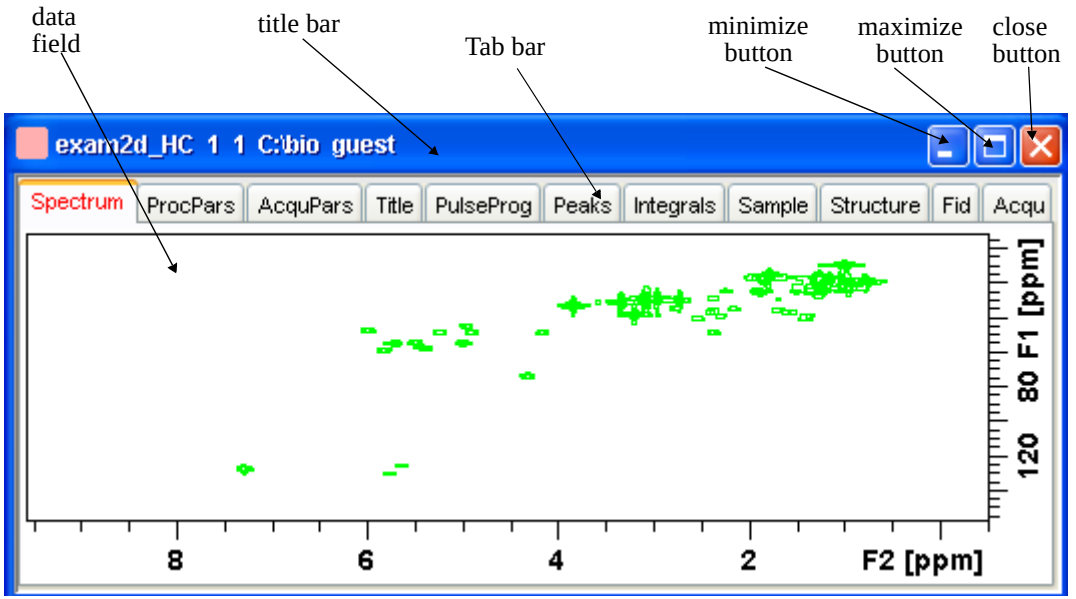


Figure 9.1

9.2 Changing the Display of a 2D spectrum

TOPSPIN offers various buttons to scale or shift a 2D spectrum both vertically and horizontally.

How to Change the Intensity Scaling (contour levels)

☞ Click the button:

Change the intensity scaling (contour levels) [***edlev***]

or

☞ Hit one of the keys:

- ***Alt***+***PageUp*** : Increase the intensity by a factor of 2.
- ***Alt***+***PageDown*** : Decrease the intensity by a factor of 2.
- ***Alt***+***Enter*** : Reset the intensity.

or

☞ Click one of the following buttons:

*2 Increase the intensity (decrease the levels) by 2 [***.2**].

*8 Increase the intensity (decrease the levels) by 8 [***.8**].

/2 Decrease the intensity (increase the levels) by 2 [**./2**].

/8 Decrease the intensity (increase the levels) by 8 [**./8**].

Reset the intensity to the last saved intensity (contour levels) [**.vr**].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

To manipulate all data windows, press the **Ctrl** key while clicking one of the above buttons.

How to Smoothly Change the Vertical Scaling (contour levels)

To change levels, multiplying all levels with the same factor:

☞ Click-hold the button and move the mouse.

or

☞ Turn the mouse wheel while the cursor is in the data window.

To change the level distance (increment), leaving the base level the same:

☞ Click-hold the *X button and move the mouse.

How to Display a Contour Levels Bar in the Data Window

1. Right-click in the data window and choose ***Display Properties...*** [**.dopt**]
2. Check ***Contour Levels Bar*** in the appearing dialog box and click ***OK*** (see Fig. 9.2)**.**

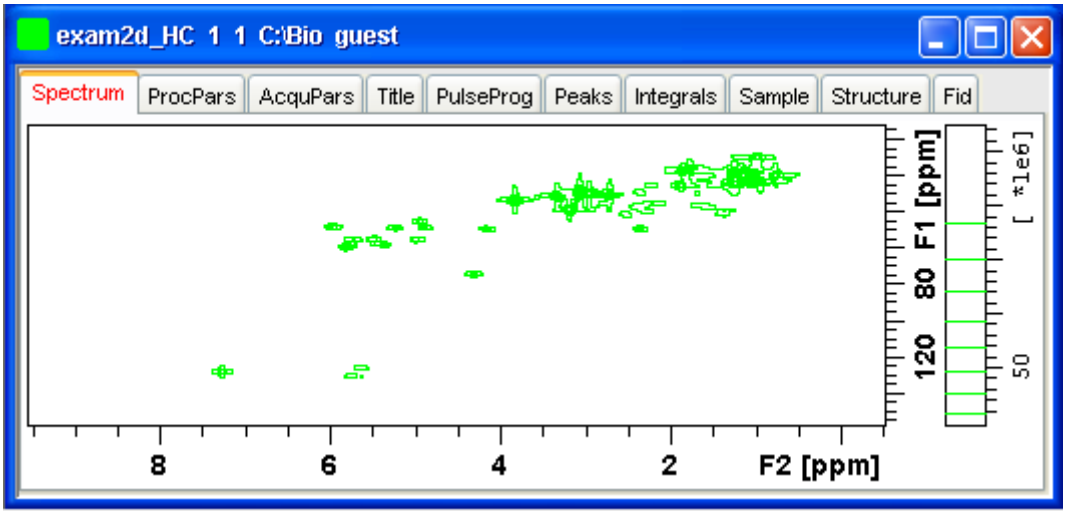


Figure 9.2

How to Switch on/off Square 2D layout

Right-click inside the data field and click ***Square Layout On/Off***

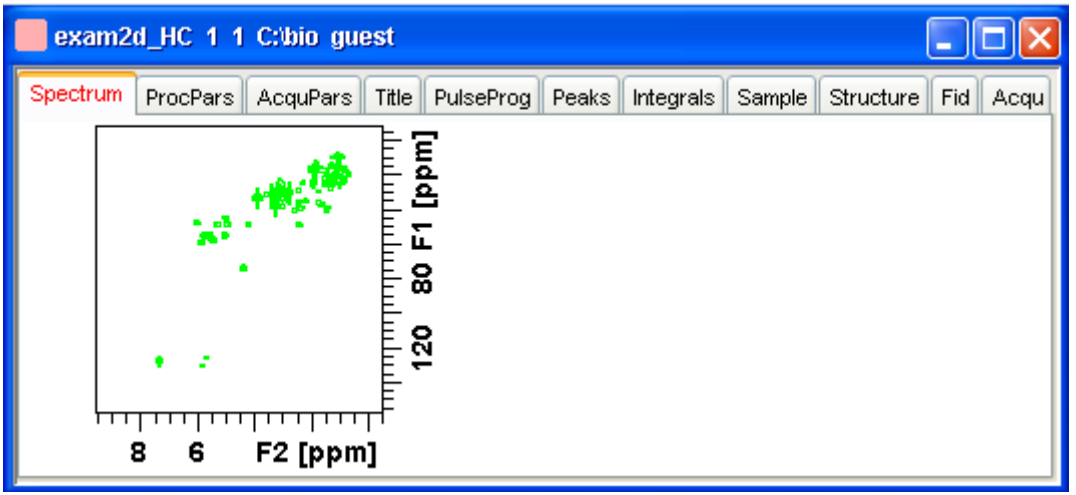


Figure 9.3

The F2 scaling will be adjusted to reach a square display.

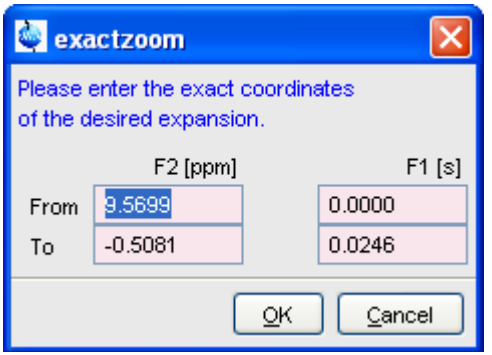
How to Zoom a 2D spectrum in/out

☞ Click one of the following buttons:

Zoom in to the center (spectrum) or left edge (FID) of the displayed region, increasing the horizontal scaling. [***.zi***]

Zoom out from the center (spectrum) or left edge (FID) of the displayed region, decreasing horizontal scaling) [***.zo***]

Perform an exact zoom via a dialog box [***.zx***].



a) Enter the coordinates of the desired region in the dialog box.

b) Click ***OK***

Undo last zoom [***.zl***].

Show full spectral width in F2 [***.f2r***].

Show full spectral width in F1 [***.f1r***].

Show full spectrum [***.all***].

Retain horizontal and vertical scaling when modifying dataset or changing to different dataset. Effects all data windows [***.keep***].

Alternatively, you can enter the corresponding commands as specified between square brackets [].

How to Shift a Spectral Region in the F2 direction (left/right)

☞ Click one of the following buttons:

- Shift to the left, half of the displayed region [***.sl***].
- Shift to the right, half of the displayed region [***.sr***].

or

☞ Click-hold the button and move the mouse:

- Smoothly shift in any direction.

Alternatively, you can enter the corresponding commands as specified between square brackets [].

How to Shift a Spectral Region in the F1 direction (up/down)

☞ Click one of the following buttons:

- Shift the spectrum up, half of the displayed region [***.su***].
- Shift the spectrum down, half of the displayed region [***.sd***].

or

☞ Click-hold the button and move the mouse:

- Smoothly shift up/down and left/right.

Alternatively, you can enter the corresponding commands as specified between square brackets [].

9.3 Show Display Properties/Regions/Files

If you right-click inside the data window, the popup menu shown in Fig. 9.4 will

appear.

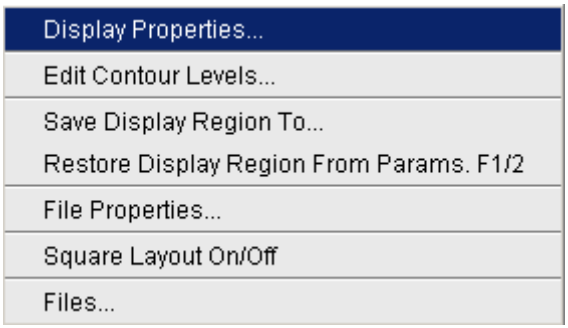


Figure 9.4

Here you can select various display properties, region setting and file properties. If you choose ***Display Properties...***, a dialog box (see Fig. 9.5) will appear.



Figure 9.5

Here you can set various display options including parameter, integrals, peaks, contours, projections and electronic signature. The number of displayed digits for the integral and peak labels can be set in the User Preferences (click ***Options*** → ***Preferences*** → ***Spectrum***).

9.4 Using the Tab bar

The 2D data window is a tabbed pane. This means its contents depends on the currently active tab in the Tab bar. The individual tabs are basically the same as for 1D display (see chapter 8.4). There are, however, some differences, which are discussed below.

How to Set Processing Parameters

☞ Click the ***ProcPars*** tab [**`edp`**]

The 2D processing parameter editor contains a column for each of the two dimensions F2 and F1 (see Fig. 9.6). Note that not all parameters exist in both dimensions.

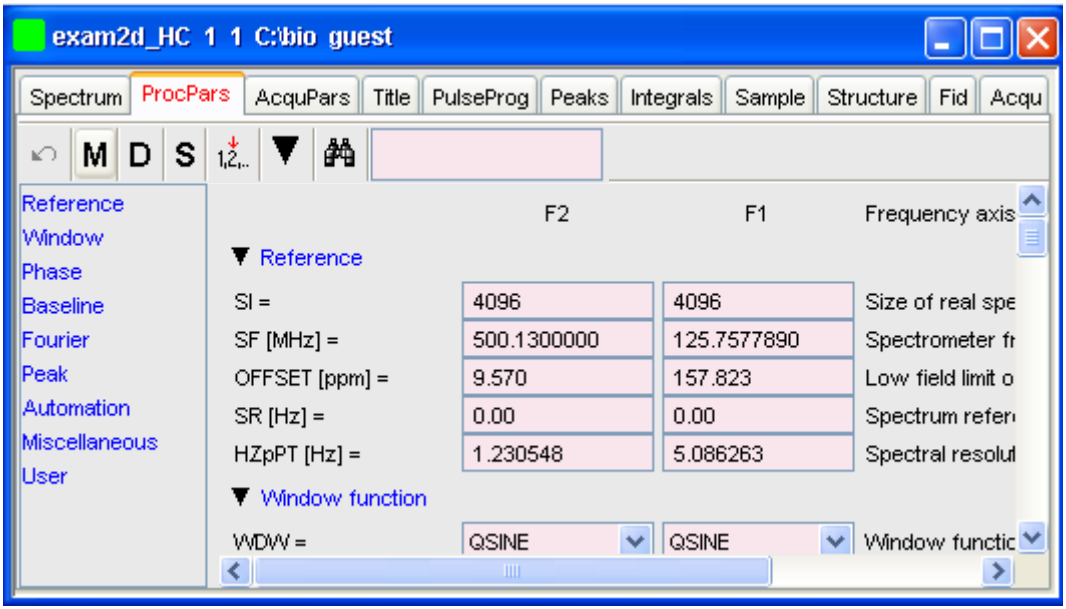


Figure 9.6

How to Set Acquisition Parameters

☞ Click the ***AcquPars*** tab [**`eda`**]

The 2D acquisition parameter editor contains a column for each of the two dimensions F2 and F1 (see Fig. 9.7). Note that not all parameters exist in both di-

mensions.

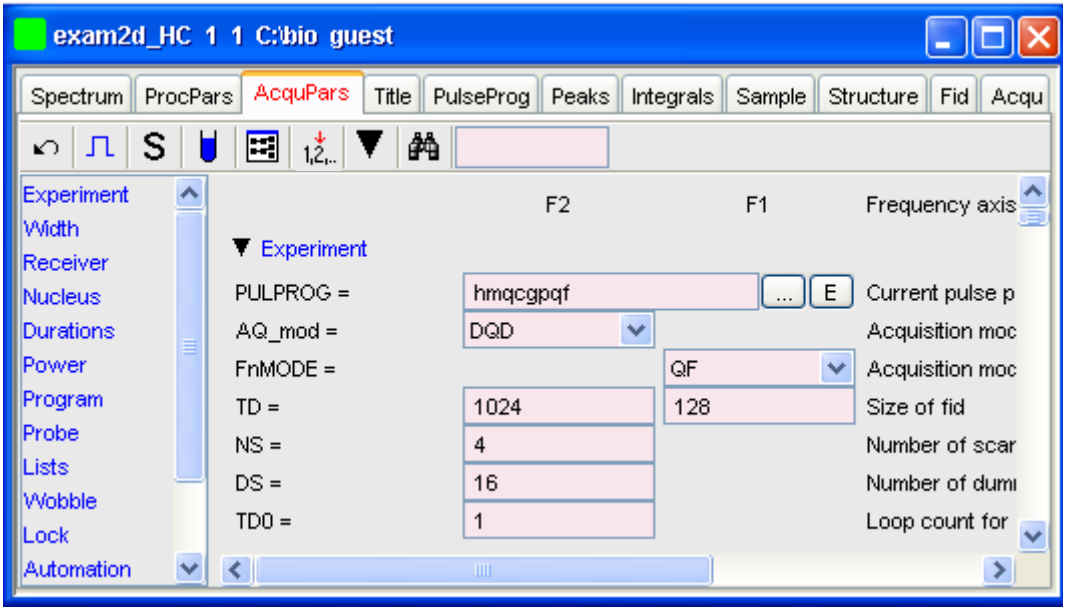


Figure 9.7

How to Display the Peak list

☞ Click the ***Peaks*** tab

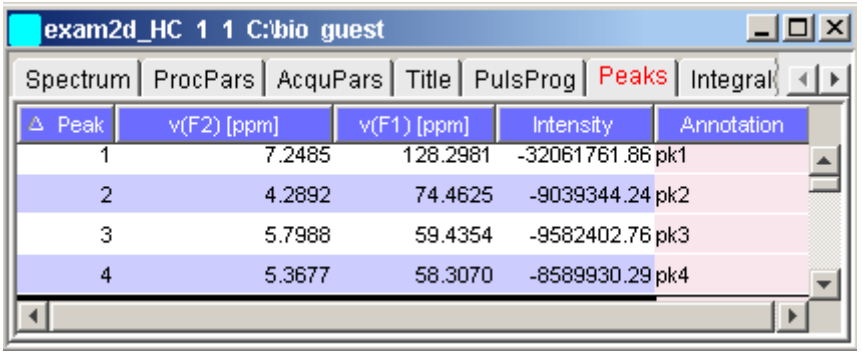


Figure 9.8

This displays list of peaks if these have been calculated (command ***pp***). The list

is basically the same as for 1D spectra. The only difference is that there are two columns for the two dimensions:

v(F2) [ppm] : the chemical shift in the F2 direction

v(F1) [ppm] : the chemical shift in the F1 direction

To specify or edit an annotation, click inside the *Annotation* field and enter a character string. The peak annotations are shown in the correlated spectrum (see Fig. 9.9)

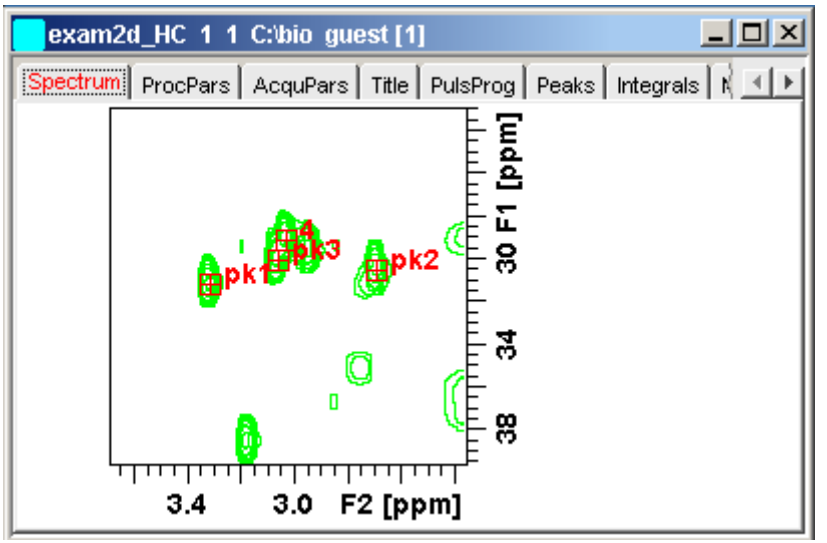


Figure 9.9

How to Display the Integral list

☞ Click the ***Integrals*** tab

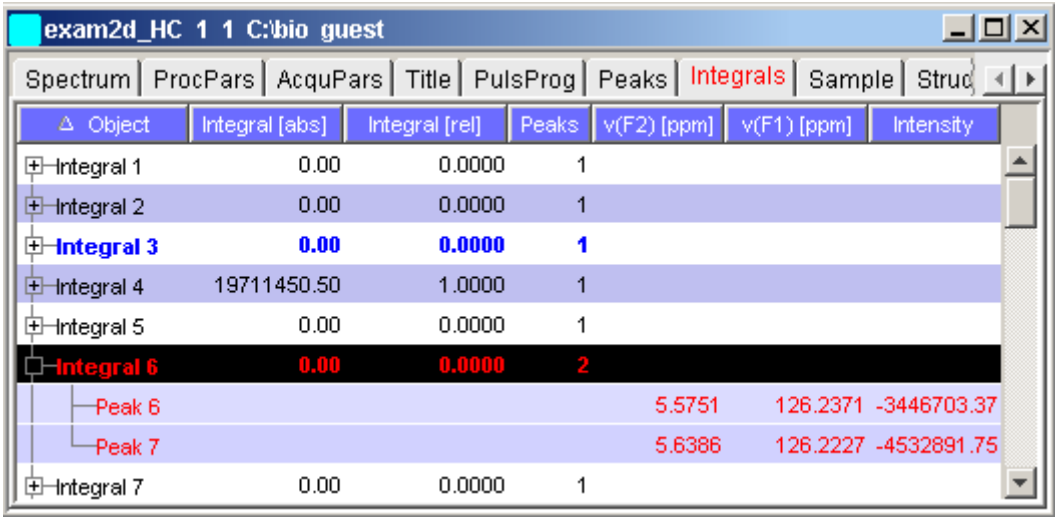


Figure 9.10

This displays list of integrals if these have been calculated (command ***int***). The list is basically the same as for 1D spectra. The only difference is that, when peaks are shown, there are two columns for the chemical shift:

v(F2) [ppm] : the chemical shift in the F2 direction

v(F1) [ppm] : the chemical shift in the F1 direction

Furthermore, a stored or exported 2D integral list can be imported as follows:

1. Right-click an entry to open the popup menu
2. Click **Import...**
3. In the appearing dialog box, navigate to the directory where the list resides and select the integral list.

As such you can import an integral list from a different dataset or a previously exported list from the current dataset. Note that integration commands store the integral list in the processed data directory under the name `integrals.txt`. Exported integrals are stored in the files `<name>.txt` and `<name>.reg`, where `<name>` is the name specified by the user.

How to Display the FID

☞ Click the ***Fid*** tab [***fid***]

2D raw data consist of a series of FIDs which are displayed in a row. Individual FIDs can be displayed by zooming in. To do that, click repeatedly. Now you can shift and zoom in/out the data to display different FIDs (see Fig. 9.11)

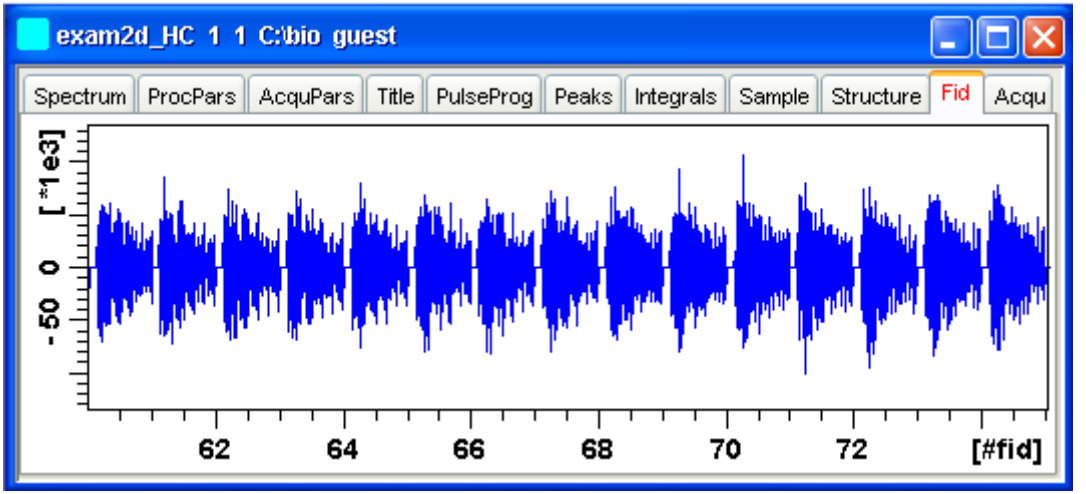


Figure 9.11

9.5 2D Display Options

How to Switch between Hertz and ppm Axis Units in F2 and F1

☞ Click the following multi-state button in the upper toolbar:

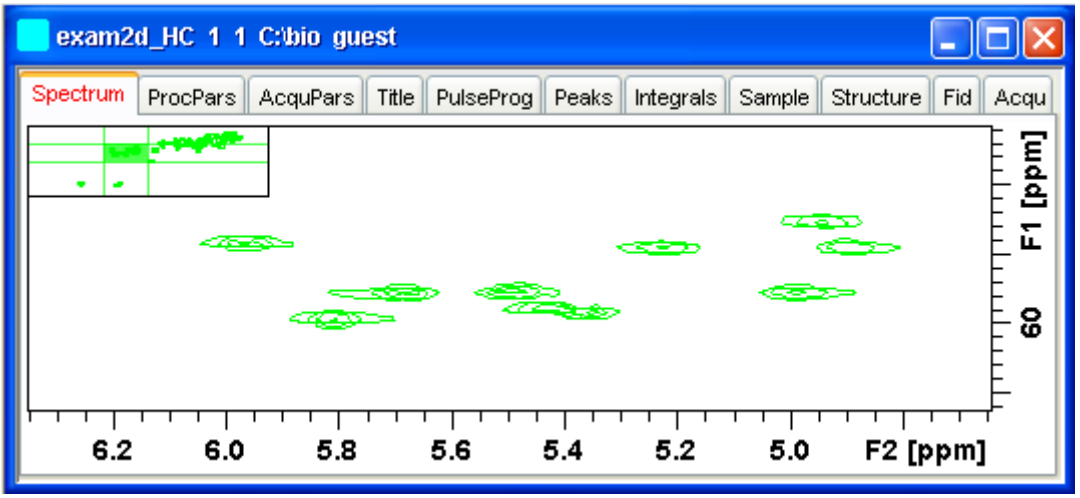
Switch between Hz and ppm axis units in F2 and F1 [**.hz**]

How to Switch on/off the Spectrum Overview display

☞ Click the following toggle button in the upper toolbar:

Switch the spectrum overview display on/off [**.ov**]

With the spectrum overview on, the data window will, for example, look like this:

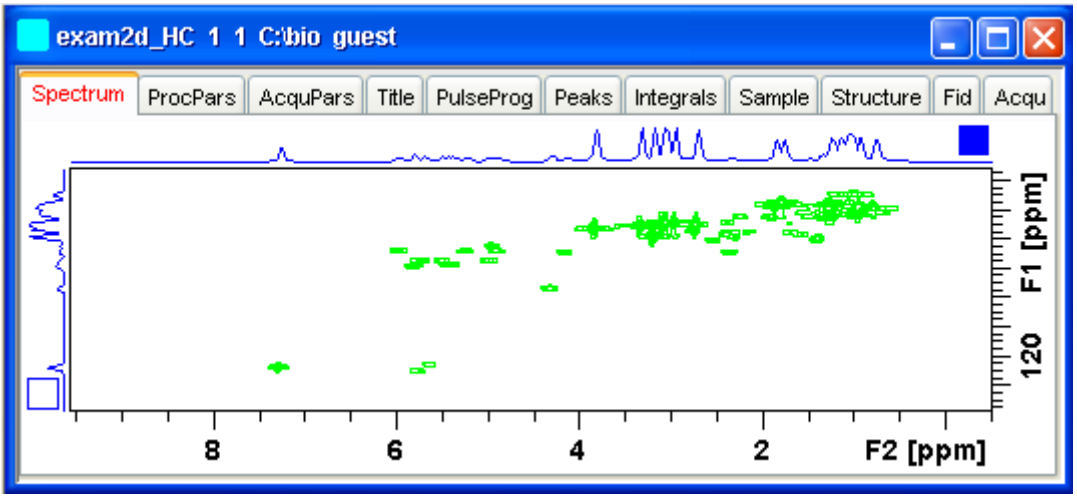


How to Switch on/off the Projection display

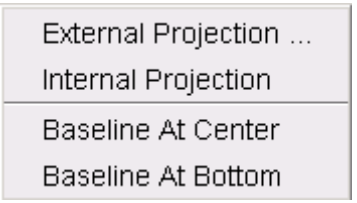
☞ Click the following toggle button in the upper toolbar:

Switch the projection display on/off [***.pr***]

With the projections displayed, a 2D dataset looks like this:



In this example, the F1 projection is selected as indicated by the filled blue square whereas the F2 projection is not selected. A selected projection can be rescaled using the toolbar rescale buttons of function keys. If you right-click inside the projection area of the data window, the following popup menu appears:



Clicking ***External Projection*** opens the a dialog box where you can specify or search for a 1D dataset and display this as a projection of the current 2D dataset.

Clicking ***Internal Projection*** calculates and displays the positive projection and displays it along with the 2D spectrum.

Clicking ***Baseline at Bottom*** or ***Baseline at Center*** allows you to put the projection baseline at the respective positions.

Alternative ways to calculate/display projections are:

☞ Right-click on a 1D dataset in the browser and choose:

Display As 2D Projection

or

☞ Click ***Processing*** → ***Calculate projections*** [***proj***]

This will open the dialog box shown in Fig. 9.12.

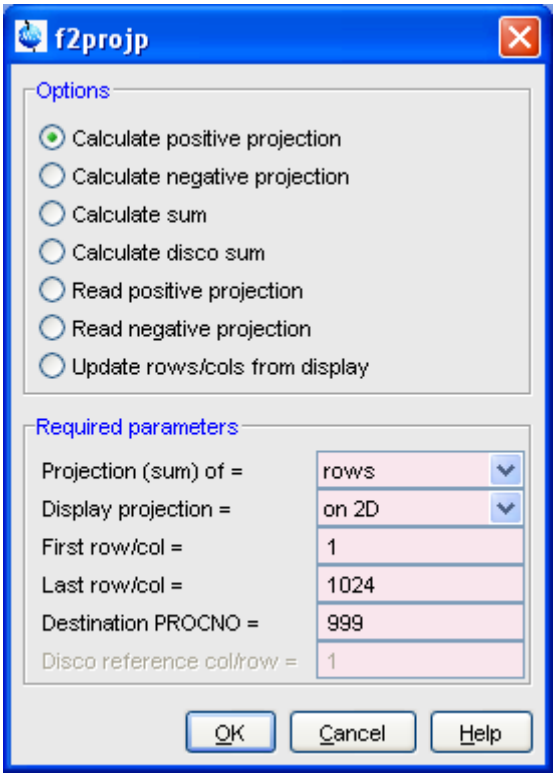


Figure 9.12

From here, you can calculate positive, negative, sum and disco projections and either show them with the 2D spectrum or display them in separate data window as a 1D data. For more details on the corresponding commands (as shown in the header of the dialog box), please refer to the Processing Reference Manual.

How to Switch on/off the Grid display

☞ Click the following multi-state button in the upper toolbar:


Switch between 'no grid', 'axis aligned grid' and 'fixed grid' [***.gr***]

Fig. 9.13 shows an example of axis aligned grid display.

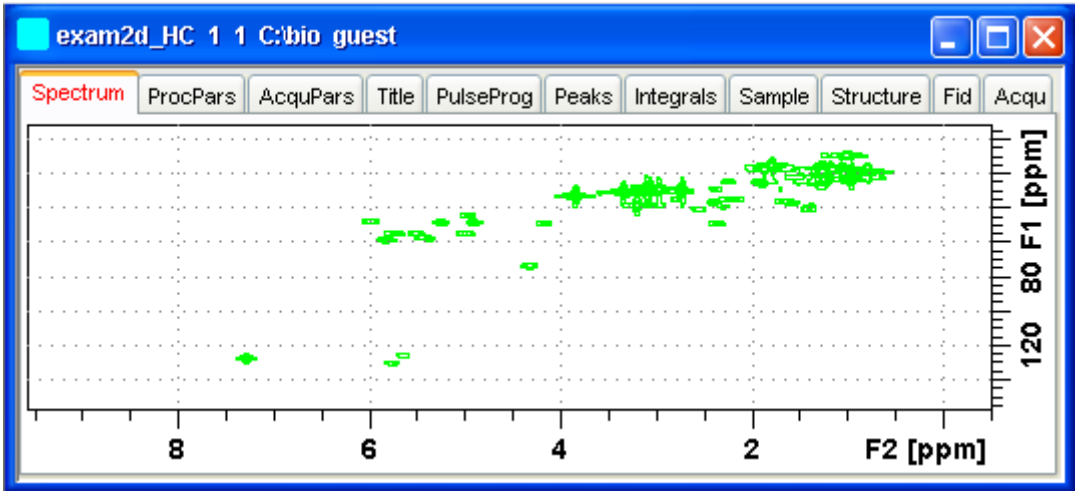


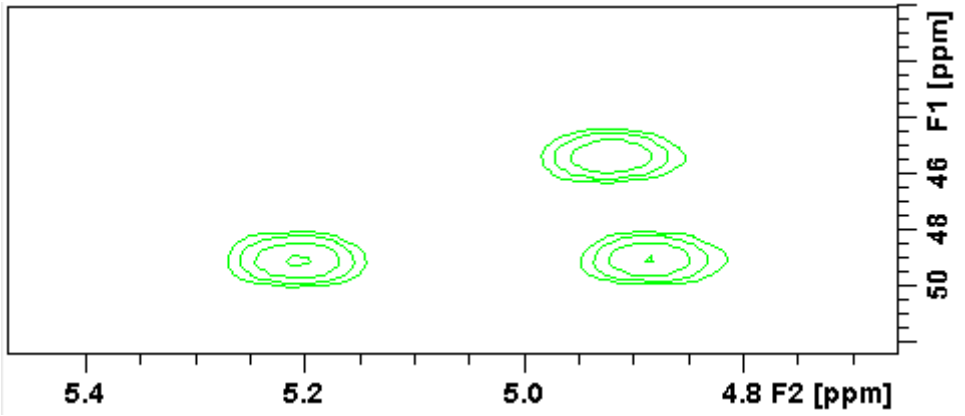
Figure 9.13 Axis aligned grid display

How to Display a 2D Spectrum in Contour Mode

☞ Click the following button in the upper toolbar:

Switch to contour display mode [**.co**]

In contour mode, a spectral region looks like this:



How to Set the 2D Contour Levels

☞ Click the following button in the lower toolbar

 Edit contour levels [***edlev***, ***.lv***]

This will open the following dialog box shown in Fig. 9.14. Contour levels can be entered manually or they can be calculated.

Manual setup

This allows you to create an arbitrary sequence of levels

1. Enter the level values in the fields 1, 2, ... at the top of the dialog box.
2. Click ***Apply*** to update the display or ***OK*** to store the levels, update the display and close the dialog box.

Calculation

This allows you to easily create a geometric or equidistant sequence of levels.

1. Click one of the following items:
   - ***Multiply with increment***
     to create a geometric sequence of levels.
   - ***Add increment***
     to create a equidistant sequence of levels.
2. Enter the desired *Base level*, *Level increment* and *Number of levels.*
3. Click ***Fill*** to display and activate the sequence.
4. Click ***Apply*** to update the display or ***OK*** to store the levels, update the display and close the dialog box.

The Contour level sign allows you to select positive levels, negative levels or both.

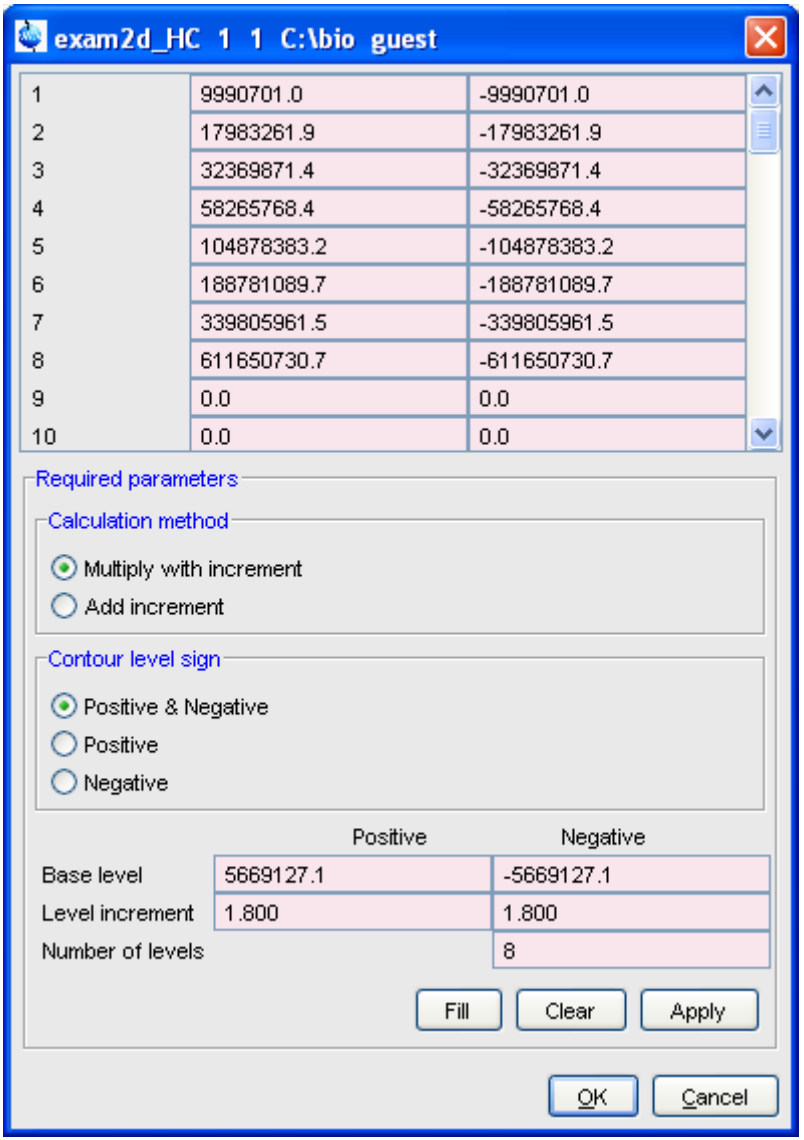


Figure 9.14

How to Store interactively set Contour Levels

To store contour levels that were set interactively, for example by clicking *2 or

pressing ***Alt***+***PageUp***:

☞ Click the following button in the lower toolbar:

Store contour levels [***.ls***]

The levels are stored in the file:

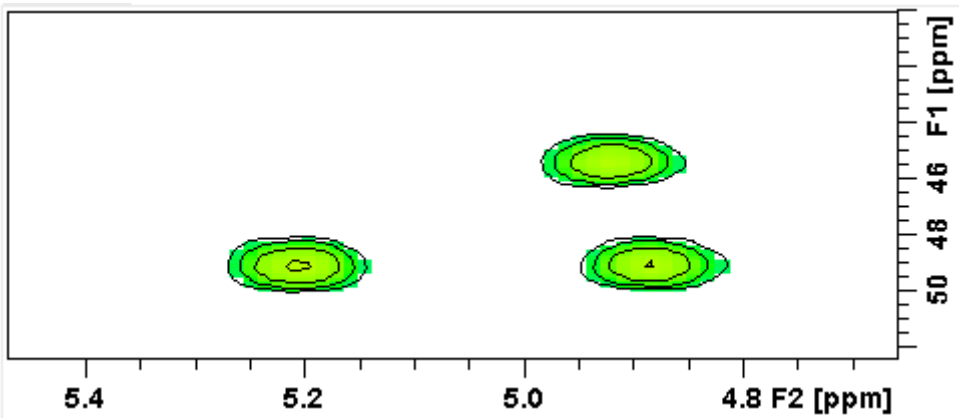
/<*dir*>/data/<*user*>/nmr/<*name*>/<*expno*>/pdata/<*procno*>/clevels

How to Display a 2D spectrum in Pseudo Color Mode

☞ Click the following button in the upper toolbar:

Switch to image color display mode [***.im***]

In pseudo color mode, a spectral region looks like this:



Note that in pseudo color mode, the contours are superimposed, in black, when you zoom in on a small region of the spectrum.

How to Display a 2D Spectrum in Oblique Mode

☞ Click the following button in the upper toolbar

Switch to oblique display mode [***.st***]

In oblique mode, a spectral region looks like in Fig. 9.15.

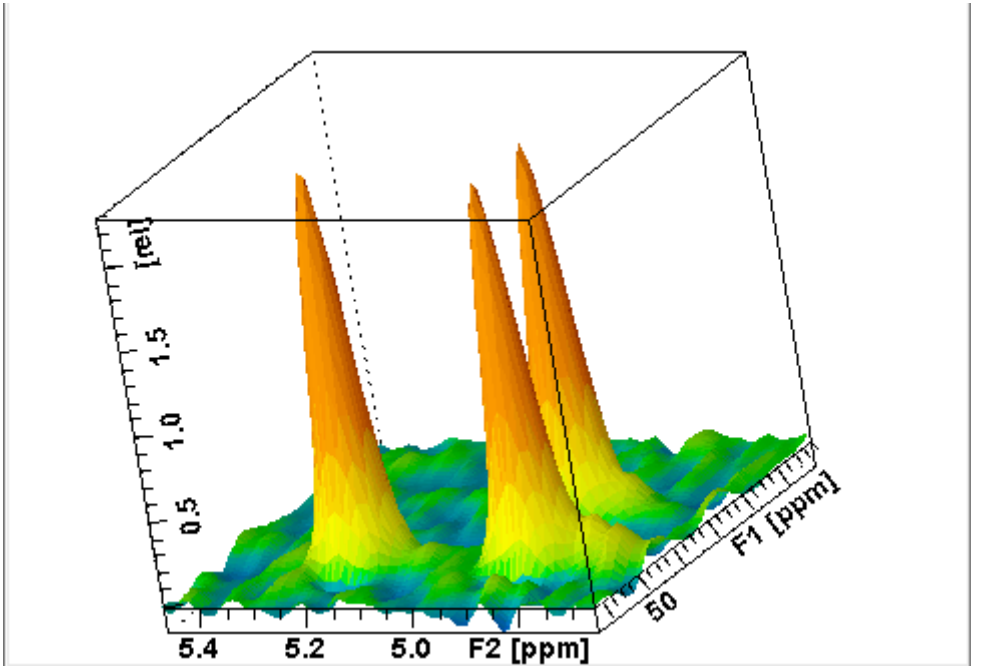


Figure 9.15

In this mode you can manipulate the display in various ways. Just right-click inside the data window and choose one of the options from the appearing popup menu (see Fig. 9.16)

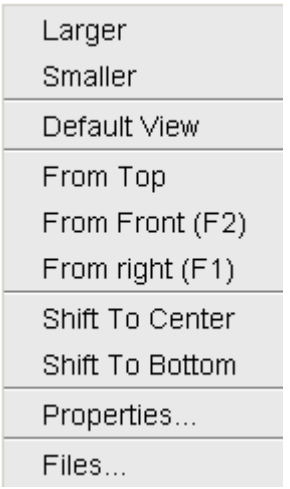


Figure 9.16

How to Rotate a 2D Spectrum in Oblique Mode

Click-hold one of the following button and move the mouse up/down:

- Rotate around x-axis.
- Rotate around y-axis.

How to Switch between Displaying Positive and Negative levels

Click the following multi-state button in the lower toolbar:

- Switch between *positive*, *negative* and *both* contours [**`.lt`**].

Chapter 10

nD Display

10.1 Display Planes of 3D Data

3D data can be displayed as 2D planes or as a 3D cube. By default, the first F3-F1 plane is displayed (see Fig. 10.1) The plane orientation and number is shown. The cube in the lower left corner graphically indicates which plane is displayed. The full 2D display functionality is available (see chapter 9).

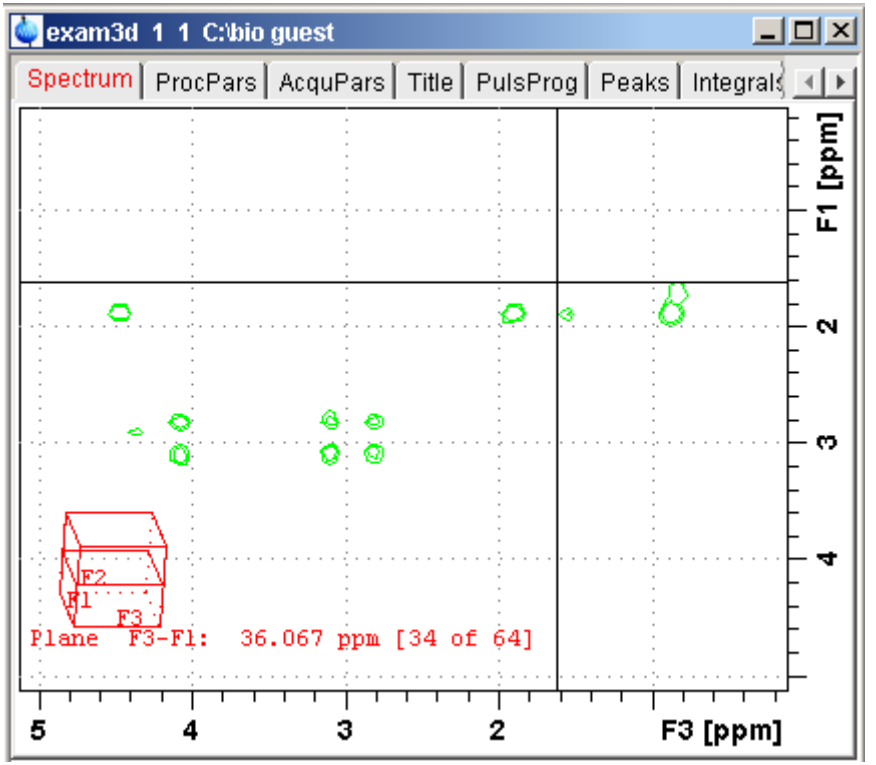


Figure 10.1

How to Switch to 2D Plane Display

If the 3D cube is displayed you can switch to 2D plane display by clicking one of the following buttons:

- Switch to 2D contour display.
- Switch to 2D image display.
- Switch to 2D oblique display.

How to Display various Plane Orientations

Click one of the following buttons:

- 12 Show F1-F2 planes.

23 Show F2-F3 planes.

31 Show F3-F1 planes.

How to Display various Plane Positions (numbers)

Click one of the following buttons:

+ Show the next plane.

− Show the previous plane.

↕ Scan planes smoothly.

E Enter the exact plane number. This will open the dialog shown in Fig. 10.2. Here, you can specify the desired plane number as well as switch to a different plane orientation.

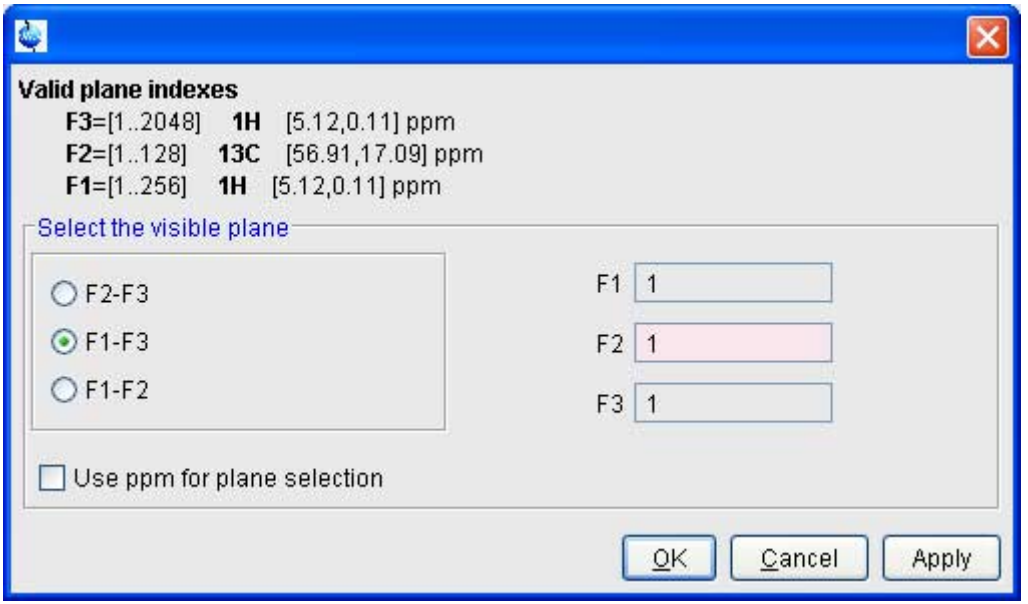


Figure 10.2

10.2 3D Cube Display Mode

How to Display the 3D Cube

Click the following button:

Show 3d cube (see Fig. 10.3).

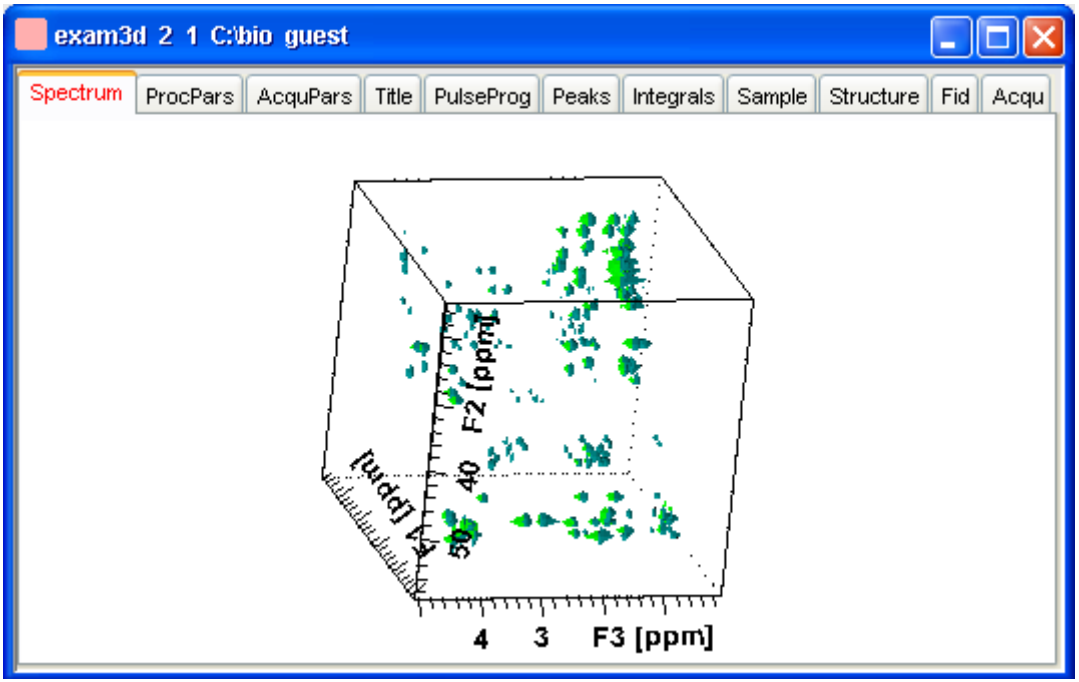


Figure 10.3

How to Rotate the 3D Cube

Click-hold one the following buttons and move the mouse up/down:

Rotate cube around x-axis.

Rotate cube around y-axis.

Rotate cube around z-axis.

How to Scale Up/Down the 3D Cube

1. Right-click inside the data window.
2. Choose ***Larger*** or ***Smaller*** from the popup menu (see Fig. 10.4).

How to Reset the Cube Size and Orientation

Click the following button:

R Reset to default size and orientation.

How to Switch Depth Cueing on/off

1. Right-click inside the data window
2. Choose ***Depth Cueing On/off*** (see Fig. 10.4)

Depth cueing makes data points which are closer to the viewer appear brighter and those that are further away appear dimmer. This increases the depth effect of the 3D image.

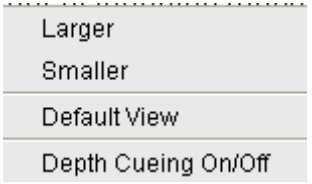


Figure 10.4

How to Display a Cube Front or Side view

Click one the following buttons:

12 Show F1-F2 plane.

23 Show F2-F3 plane.

31 Show F3-F1 plane.

10.3 nD parameter display

TOPSPIN 2.1 and newer support parameter display of up to 8D data. To show processing parameters:

☞ click the ***ProcPars*** tab of the data window

or

☞ enter ***edp*** on the command line

Parameters of each direction are shown in a separate column. Fig. 10.5 shows the

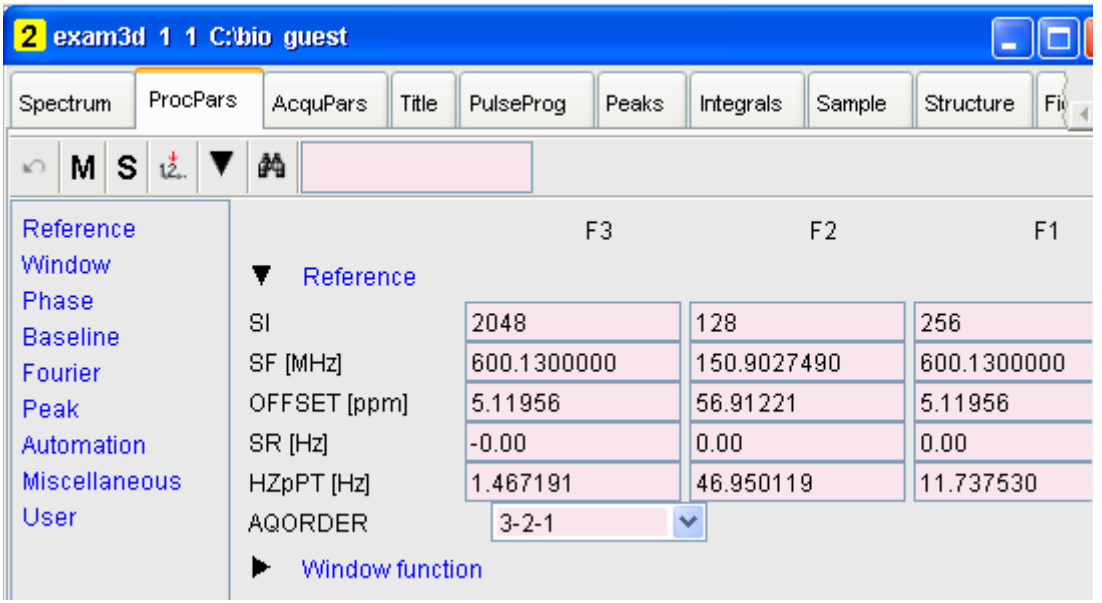


Figure 10.5

processing parameter display of a 3D dataset.

To show acquisition parameters:

☞ click the ***AcquPars*** tab of the data window

or

☞ enter ***eda*** on the command line

Parameters of each direction are shown in a separate column. Fig. 10.5 shows the

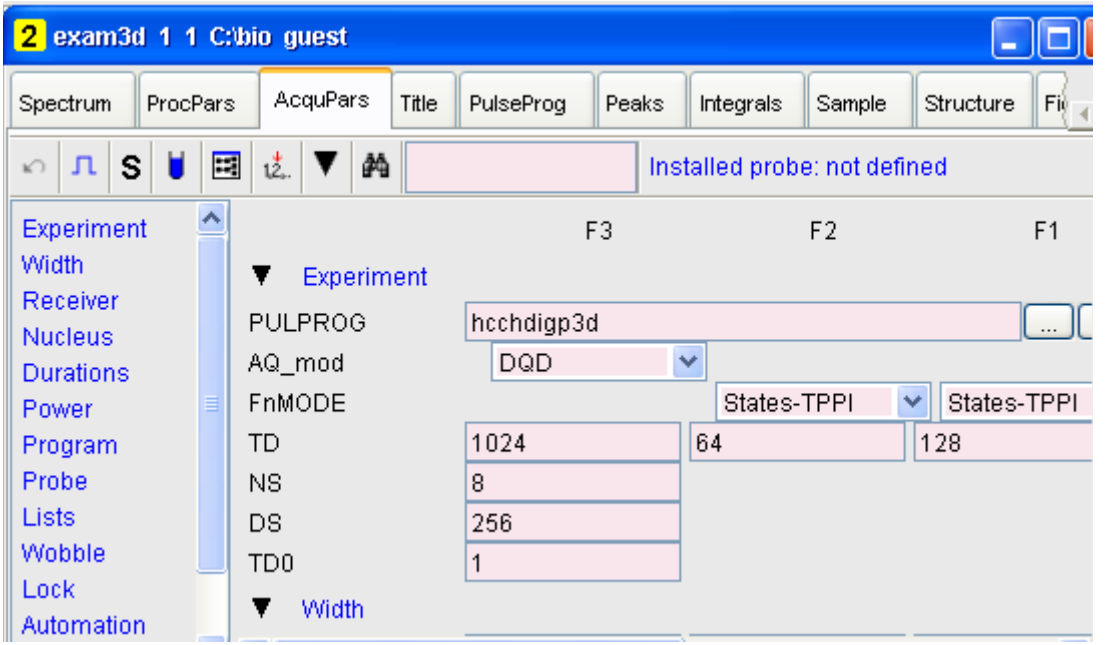


Figure 10.6

acquisition parameter display of a 3D dataset.

10.4 nD Fid Display

nD raw data can be displayed as a series of 1D FIDs. To do that:

☞ click the ***FID*** tab of the data window

or

☞ enter ***`fid`*** on the command line

10.5 nD Peak and Integral Display

TOPSPIN 2.1 and newer support peak and integral display of up to 8D data.

To show the nD peak list:

☞ click the ***Peaks*** tab of the data window

or

☞ enter ***peaks*** on the command line

Fig. 10.7 shows the peak list of a 3D dataset.

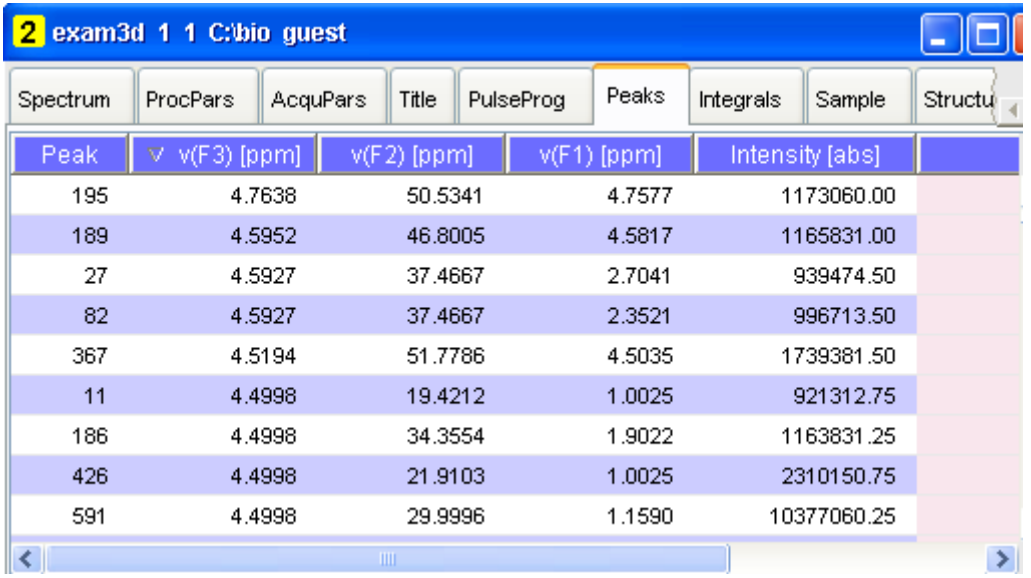


Figure 10.7

The chemical shift in each of the three dimensions is shown in a separate column.

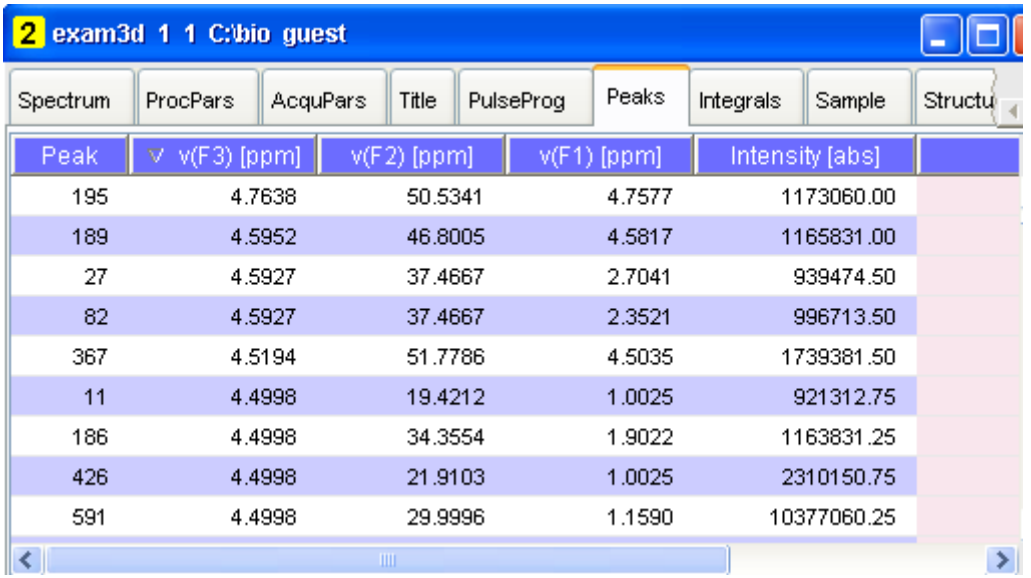
To show the nD integral list:

☞ click the ***Integrals*** tab of the data window

or

☞ enter ***ints*** on the command line

Fig. 10.7 shows the integral list of a 3D dataset.



Peak	v(F3) [ppm]	v(F2) [ppm]	v(F1) [ppm]	Intensity [abs]
195	4.7638	50.5341	4.7577	1173060.00
189	4.5952	46.8005	4.5817	1165831.00
27	4.5927	37.4667	2.7041	939474.50
82	4.5927	37.4667	2.3521	996713.50
367	4.5194	51.7786	4.5035	1739381.50
11	4.4998	19.4212	1.0025	921312.75
186	4.4998	34.3554	1.9022	1163831.25
426	4.4998	21.9103	1.0025	2310150.75
591	4.4998	29.9996	1.1590	10377060.25

Figure 10.8

The chemical shift in each of the three dimensions is shown in a separate column.

Peaks and integrals only appear if they have been calculated (commands ***pp*** and ***int***, respectively)..

Chapter 11

1D Interactive Manipulation

The upper toolbar of the 1D menu offers various buttons for interactive manipulation. If you click such a button, the active data window will switch to the corresponding mode. An interactive manipulation mode is data window specific, i.e. it only applies to the active window.

11.1 1D Interactive Window multiplication

TOPSPIN 2.0 and newer supports 1D interactive window multiplication.

11.1.1 1D Interactive Window Multiplication Procedure

How to Switch to Window Multiplication Mode

☞ Click the ***Processing*** → ***Window Multiplication*** [**wm**], enable **Manual window adjustment** in the appearing dialog and click ***OK***.

or

☞ Enter **.winf** on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig. 11.2) and the data window itself will be divided into three parts:

- a parameter part at the left

- a spectrum part at the upper right
- a FID part at the lower right.

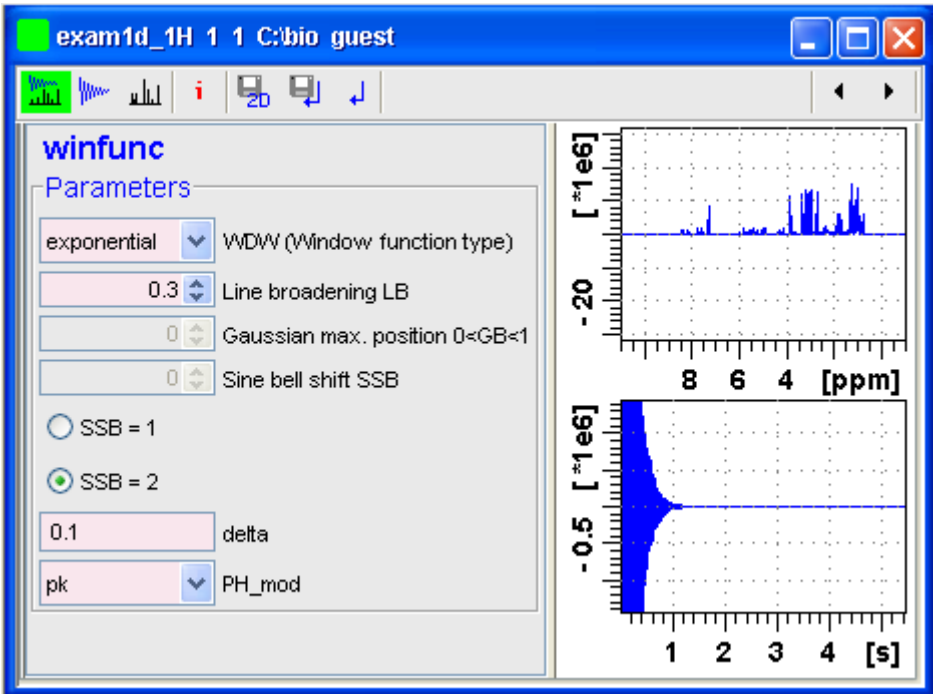


Figure 11.1

Show both spectrum and FID.

Show FID only.

Show spectrum only.

Switch cursor information on/off (toggle)

Save windows settings to source 2D dataset[1] and return.

1. 2D data from which current 1D dataset was extracted, e.g. with ***rser***.

 Save window settings and return

 Return without save.

You can perform interactive window manipulation as follow:

1. Select the window function (parameter WDW)
2. Set the corresponding parameter(s), e.g.
   - LB for exponential
   - LB and GB for Gaussian
   - SSB for sine bell and squared sine

   The displayed spectrum and/or FID will be automatically adjusted as you change the window function and parameters.
3. Click  to store the window settings and return.

Now you can perform further processing steps like Fourier transform, phase correction etc.

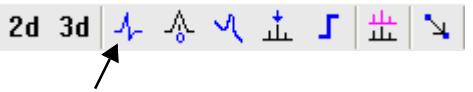
11.2 1D Interactive Phase Correction

Manually acquired spectra can be phased corrected automatically, with commands like ***apk*** or ***apks*** or, interactively, in phase correction mode.

11.2.1 1D Interactive Phase Correction Procedure

How to Switch to Phase Correction Mode

Click the indicated button in the upper toolbar:



or enter ***.ph*** on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig. 11.2)

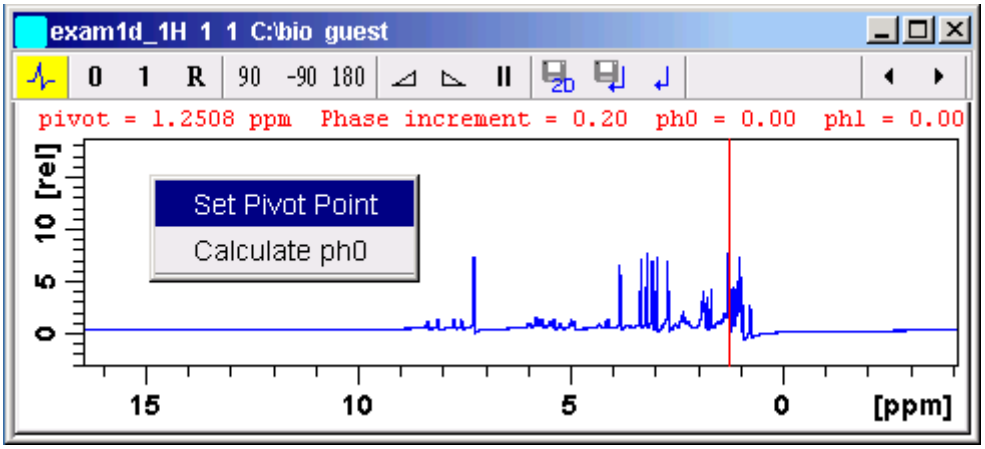

exam1d_1H 1 1 C:\bio guest
0 1 R 90 -90 180
pivot = 1.2508 ppm Phase increment = 0.20 ph0 = 0.00 ph1 = 0.00
Set Pivot Point
Calculate ph0
0 5 10 [rel]
15 10 5 0 [ppm]

Figure 11.2 Data window in phase correction mode

The yellow button indicates that you are in phase correction mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

How to Perform a Typical 1D Interactive Phase Correction

For a typical 1D phase correction, take the following steps:

1. Click-hold the button **0** and move the mouse until the until the reference peak is exactly in absorption mode.
2. Click-hold the button **1** and move the mouse until the entire spectrum is exactly in absorption mode.
3. Click the button to save and execute the phase correction and return.

11.2.2 1D Interactive Phase Correction Details

How to Set the Phase Pivot Point

By default, the phase pivot point is set to the biggest magnitude intensity of the displayed region of the spectrum. To change the pivot point:

1. Right-click on the desired pivot point position
2. Choose ***Set pivot point*** from the popup menu (see Fig. 11.2)

How to Perform Default Zero Order Phase Correction

1. Right-click in the data window
2. Choose ***Calculate ph0*** in the popup menu (see Fig. 11.2)

The spectrum will automatically be corrected according to the calculated value.

How to Perform Interactive Zero Order Phase Correction

1. Click-hold the following button (button turns green):

   0 Zero order phase correction (parameter PHC0).

2. Move the mouse until the reference peak is exactly in absorption mode.
3. Release the mouse (button turns grey).

How to Perform Interactive First Order Phase Correction

1. Click-hold the following button (button turns green):

   1 First order phase correction (parameter PHC1).

2. Move the mouse until the entire spectrum is exactly in absorption mode.
3. Release the mouse (button turns grey).

How to Perform 90, -90 or 180° Zero Order Phase Correction

☞ Click one of the following buttons:

90 Perform 90 zero order phase correction [***.ph90***].

-90 Perform -90° zero order phase correction [***.phm90***].

180 Perform 180° zero order phase correction [***.ph180***].

How to Reset the Phase to the Original Values

☞ Click the following button:

R Reset zero and first order phase values [***.phr***].

How to Change the Mouse Sensitivity

☞ Click one of the following buttons:

 Increase (double) the mouse sensitivity [***.inc***].

 Decrease (halve) the mouse sensitivity [***.dec***].

 Reset the mouse sensitivity.

How to Return from Phase Correction Mode with/without Save

To return while saving the phase correction to the current dataset:

☞ Click the following button:

 Save, execute and return [***.sret***].

This will perform the following tasks:

- Execute phase correction (command ***pk***).
- Save the current phase correction values.
- Leave the phase correction mode.

To return without save:

☞ Click the following button:

 Return, discarding any changes [***.ret***].

To return while saving the phase correction to the source 2D dataset:

☞ Click the following button:

 Save to 2D [***.s2d***].

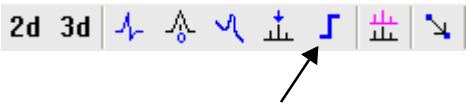
This is only applicable on rows or columns extracted from 2D data. The phase values will be saved to the 2D dataset from which the current 1D dataset was extracted.

11.3 1D Interactive Integration

Integration of 1D data can be done automatically, with the commands ***abs*** and ***li*** or, interactively, as described in this paragraph.

How to Switch to Integration Mode

☞ Click the indicated button in the upper toolbar:



or enter ***.int*** on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig. 11.3). The first button (define integrals) is automatically activated (is green).

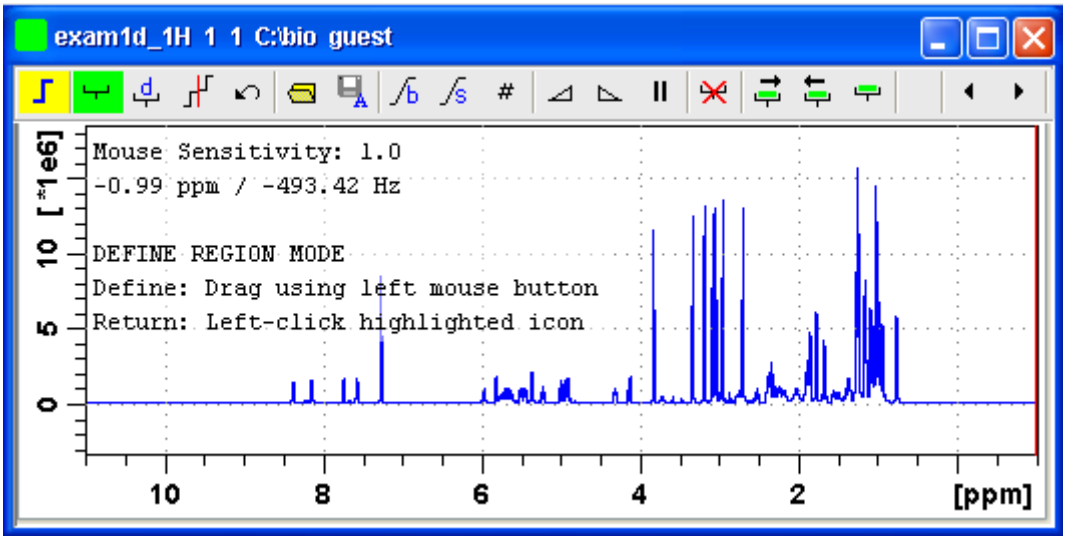


Figure 11.3 Data window in integration mode

The yellow button indicates that the data window is in integration mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

If integral regions have already been determined, for example with ***abs*** or with a previous interactive integration, these regions are displayed in the data window, along with the integral values. You can remove them, change them or add to them, as described below.

How to Define Integral Regions

To define integral regions interactively:

1. Click the following button (button turns green):

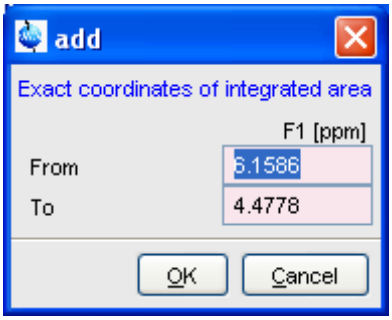
   Define integral region interactively.

   Note that the define integrals button is automatically activated on entering the integrals mode.
2. Put the red cursor line at one edge of a peak or multiplet.
3. Left-click-hold and drag the cursor line to the other edge of the peak or multiplet.
4. Do step 2 and 3 for all regions to be defined.
5. Click the green button to leave the "define region" mode (button turns grey).

To define integral regions via a dialog box:

1. Click the following button:

   Define region via dialog.
2. In the appearing dialog box:



   Enter the exact values for the region limits.
3. Click ***OK*** to define the selected region.

How to Select/Deselect Integral Regions

To select/deselect <u>all displayed</u> integral regions:

☞ Click the button: button

To select a single integral region:

1. Right-click in the integral region.
2. Choose ***Select/Deselect*** from the popup menu.

To select the next integral region:

☞ Click the  button

To select the previous integral region:

☞ Click the:  button.

To select multiple integral regions:

1. Click the button:  button to select all integrals
2. Deselect the integral that are not to be selected.

Selected integral regions are indicated by a color filled integral label. In the Fig. 11.4, the five left most regions are selected, the region around 6 ppm is currently being deselected.

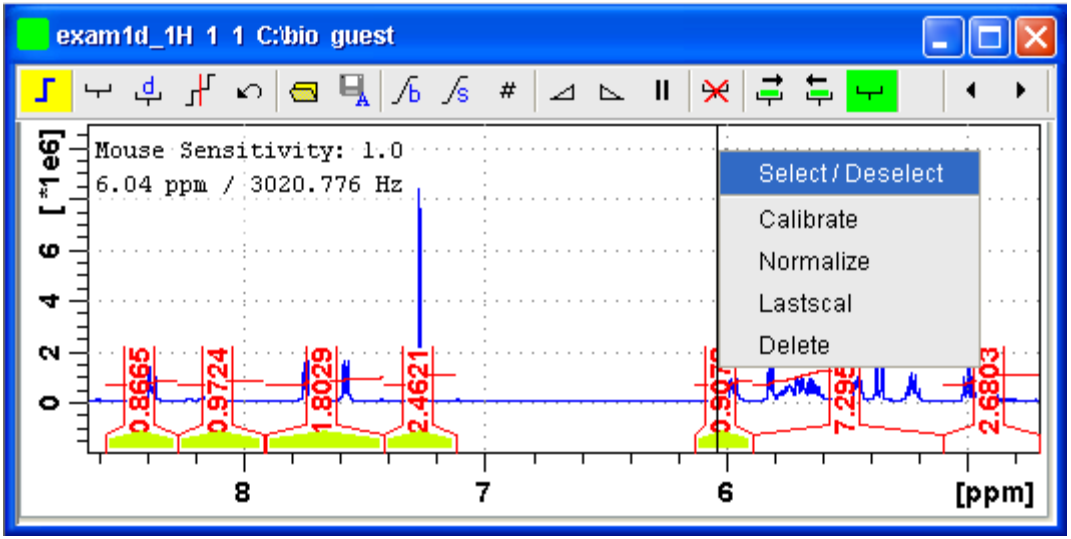


Figure 11.4

Note that:

- If no integral is selected, the next and previous integral button select the first or last integral respectively.
- the select all integrals button remains green while all or multiple integrals are selected. This indicated a selection mode.

How to Read Integral Regions from Disk

You can read integrals regions from disk which have been stored by automatic integration (command ***abs***) or by a previous interactive integration.

To read integrals:

1. Click the following button:

 Read integral regions.

The following popup menu will appear:

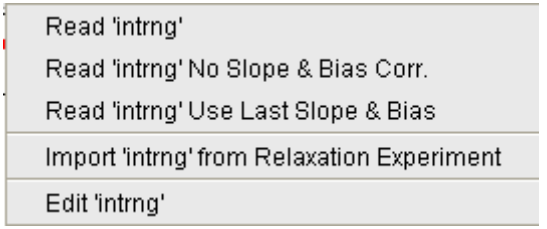

Read 'intrng'
Read 'intrng' No Slope & Bias Corr.
Read 'intrng' Use Last Slope & Bias
Import 'intrng' from Relaxation Experiment
Edit 'intrng'

Figure 11.5

2. From the popup menu, choose one of the following entries:

- ***Read 'intrng'***
  to read the last saved integral regions and apply the saved slope and bias correction values.
- ***Read 'intrng' no slope & bias corr.***
  to read the last saved integral regions but do not apply the saved slope and bias correction values.
- ***Read 'intrng' use last slope & bias***
  to read the last saved integral regions applying the last slope and bias correction values.

- ***Read 'intrng' from Relaxation Experiment***
  to read the last stored integral regions of the T1/T2 relaxation experiment.
- ***Edit 'intrng'***
  to edit the file (`intrng`) that contains the integral regions and slope and bias correction values. Changes in this file are automatically shown on the screen.

How to Perform Interactive Bias and Slope Correction

To perform interactive bias correction:

1. Select the integral(s) that you want to correct (right-click in the region).

   If no integral is selected, bias correction will work on all integrals.
2. Click-hold the following button (it turns green) and move the mouse,

   Integral bias correction.

   until the integral bias is correct.
3. Release the mouse (button turns grey).

To perform interactive slope correction:

1. Select the integral(s) that you want to correct (right-click in the region).

   If no integral is selected, slope correction will work on all integrals.
2. Click-hold the following button (it turns green) and move the mouse,

   Integral slope correction.

   until the integral slope is correct.
3. Release the mouse (button turns grey).

How to Set the Limit for Bias Determination

☞ Click the following button:

Limit for bias determination.

How to Change the Mouse Sensitivity

☞ Click one of the following buttons:

Increase (double) the mouse sensitivity [***.inc***].

Decrease (halve) the mouse sensitivity [***.dec***].

Reset the mouse sensitivity.

How to Calibrate/Normalize Integrals

Calibrating integrals means setting the value of a reference integral and adjusting all other integrals accordingly. To do that:

1. Right-click in the reference integral region.
2. Choose **Calibrate** from the popup menu (see Fig. 11.6).
3. Enter the desired value for the reference integral and click ***OK***

Normalizing integrals means setting the sum of all integrals and adjusting individual integral values accordingly. To do that:

1. Right-click in the reference integral region.
2. Choose **Normalize** from the popup menu (see Fig. 11.6).
3. Enter the desired sum of all integrals and click ***OK***

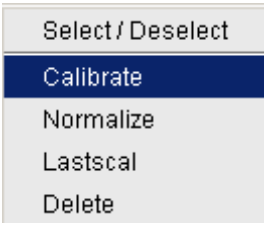


Figure 11.6

Calibrating and normalizing only effects the current dataset. To scale integrals with respect to a reference dataset, choose ***lastscal*** from the right/click popup menu (see below).

How to Scale Integrals with respect to Different Spectra

Integrals can be scaled with respect to the last spectrum that was integrated interactively. To do that:

1. Right-click in the reference integral region.
2. Choose ***Lastscal*** from the popup menu (see Fig. 11.6).

As such, you can compare integrals of different spectra. Note that this only make

sense for spectra which have been acquired under the same experimental conditions. The scaling factor is stored in the file:

```
<tshome>/prog/curdir/<user>/intscale
```

How to Delete Integral Regions from the Display

To delete the selected integral regions from the display:

☞ Click the following button:

Delete selected integral regions from the display.

To delete a single integral region from the display:

1. Right-click in the integral region.
2. Choose **Delete** from the popup menu (see Fig. 11.6)

To delete all integral regions from the display:

☞ Click the following buttons:

Select all integral regions.

Delete selected integral regions from the display.

Note that regions are only deleted from the screen. Regions which are saved on disk (in the `intrng` file) are not affected.

How to Scale Selected Integrals

Integral scaling only manipulates selected integrals. However, if no integrals are selected, it works on all integrals.

☞ Click one of the following buttons:

*2 Scale up selected integrals by a factor of 2.

/2 Scale down selected integrals by a factor of 2.

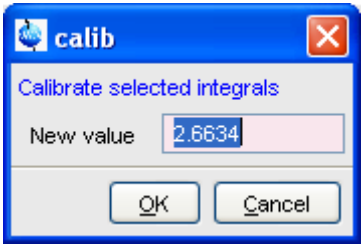
Scale selected integrals up/down smoothly.

To scale up/down integrals by a factor entered via a dialog:

1. Click the following button:

*X Scale integrals via a dialog.

2. Enter a scaling factor, e.g. 2.5. in the appearing dialog.



3. Click ***OK*** to apply this factor.

To scale all integrals to the same height:

☞ Click the following button:

= Scale/unscale all integrals to the same height.

The individual scaling factor for each region is displayed above the integral. Clicking this button again rescales all integrals to their original height.

How to Move the Integral Trails Up/Down

To move the integrals (selected and unselected) up or down:

☞ Click one of the following buttons:

↓ The left edge of the selected integral is put just above the baseline. If no integral is selected, the lowest integral is used.

↑ The right edge of the selected integral is put at 3/4 of the window height. If no integral is selected, the highest integral is used.

↕ Shift all integral trails up/down smoothly.

How to Cut Integral Regions

1. Click the following button (button turns green):

Cut integral region.

2. Move the red cursor line into an integral region to the position where it must be cut and click the left mouse button.
3. Do step 2 for each integral region that must be cut.

4. Click the (green) button to leave the *cut integral* mode (button turns grey).

In case of overlapping integrals, you must select the integral to be cut before you actually cut it.

How to Save Integral Regions

1. Click the following button:

    Save integral regions.

   The following popup menu will appear:

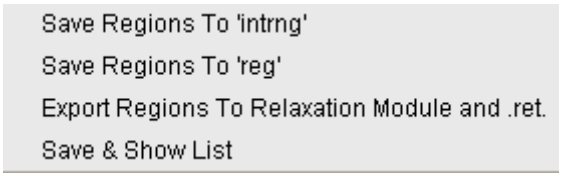


Figure 11.7

2. Choose one of the following entries:

   - ***Save regions to 'intrng'***
     Save the currently displayed integral regions including the slope and bias correction values.
   - ***Save Regions to 'reg'***
     Save the integral regions to the file `reg`.
   - ***Export Regions To Relaxation Module and .sret***
     Used on relaxation data only. Exports the integral regions for T1/T2 relaxation analysis and exits from integration mode.
   - ***Save & show list***
     Save the currently displayed integral regions including the slope and bias correction values and show the integrals on the screen.

How to Undo the Last Region Operation

☞ Click the following button:

 Undo the last region operation.

How to Return from the Integration Mode with/without Save

To return and save the integrals to the current dataset:

☞ Click the following button:


Save integrals and return [***.sret***].

As such, you will:

- save the integral regions and corresponding slope and bias corrections to the file `intrng`.
- save the integral regions, slope and bias corrections and integral values to the file `integrals.txt`. This file is displayed when you click the ***Integrals*** Tab.
- leave the integration mode.

To return without save:

☞ Click the following button:

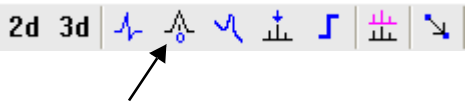

Return, discarding any changes [***.ret***].

11.4 1D Interactive Calibration

A 1D spectrum can be calibrated (referenced), automatically, with the command ***sref*** or, interactively, as described below.

How to Switch to Calibration Mode

☞ Click the indicated button in the upper toolbar



or enter ***.cal*** on the command line. The Tab bar of the active data window will be replaced by a toolbar.

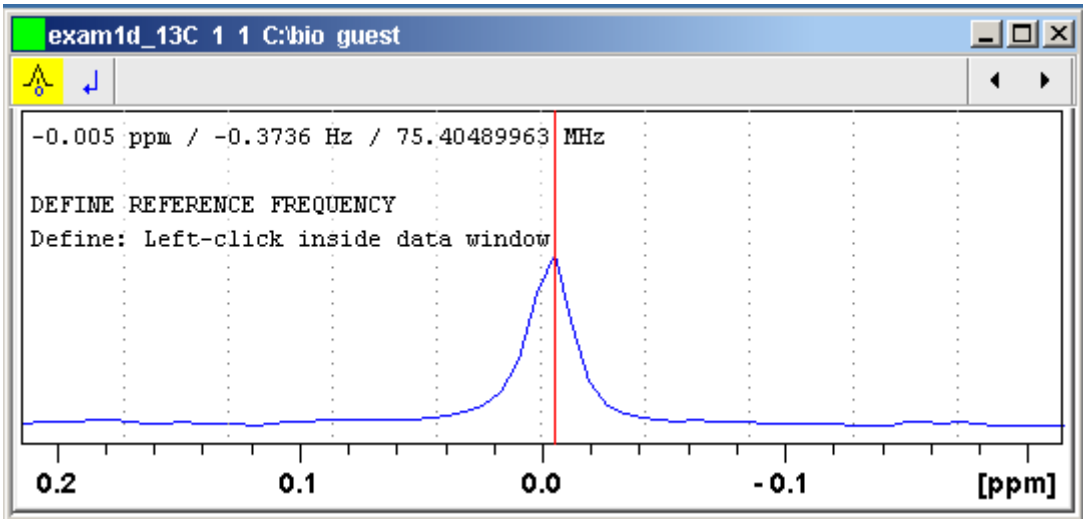


Figure 11.8 Data window in calibration mode



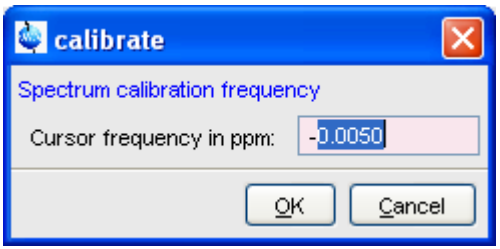
The yellow button indicates that the data window is in calibration mode.

How to Calibrate a Spectrum Interactively

In calibration mode:

1. Position the red cursor line at the reference peak.
2. Left-click at that position.

   The following dialog box will appear:



   Note that the units (Hz or ppm) correspond to the axis units of the display.
3. Enter the frequency you want to assign to the reference peak.

4. Click ***OK***

The spectrum will be calibrated and re-displayed. TOPSPIN will automatically leave calibration mode.

11.5 1D Multiple Display

The multiple display mode allows you to display multiple superimposed spectra.The spectra will be ppm aligned or Hz aligned, according to the selected axis unit. Each spectrum can be individually shifted and scaled allowing exact alignment of corresponding peaks in different spectra. The number of superimposed spectra is unlimited.

Although multiple display is normally used for spectra with matching nuclei, it allows you to superimposed spectra with non-matching nuclei. You will get a warning that the nuclei do not match. Just just click ***OK*** to continue.

How Switch to Multiple Display Mode and Read Multiple Spectra

One way to superimpose data in multiple display is to read one dataset, switch to multiple display mode and add other datasets:

1. Read a 1D dataset.
2. Click the  button in the upper toolbar or type ***.md*** on the command line.

   The data window will switch to multiple display mode.
3. Add a dataset as follows:

   ☞ Left-click-hold the dataset in the browser and drag it into the data window.

   or

   ☞ Right-click the dataset in the browser and choose ***Display*** from the popup menu.

   or

   ☞ Enter ***re*** and specify the additional dataset in the appearing dialog box.

Another way to superimpose data in multiple display is to read multiple datasets simultaneously:

1. In the browser:

☞ Hold down the ***Ctrl*** key and click multiple datasets to select them.

or

☞ Hold down the ***Shift*** key and click two datasets to select these two and all datasets in between.

2. Right-click any of the selected data:

☞ Choose ***Display*** from the popup menu.
This will show the data in the active data window if that is in multiple display mode or, otherwise, show the data in a new window.

or

☞ Choose ***Display in new window*** from the popup menu.
This will show the data in a new window.

In multiple display mode, the Tab bar of the active data window is replaced by a toolbar. Fig. 11.9 shows three comparable 1D spectra and the sum of all three.

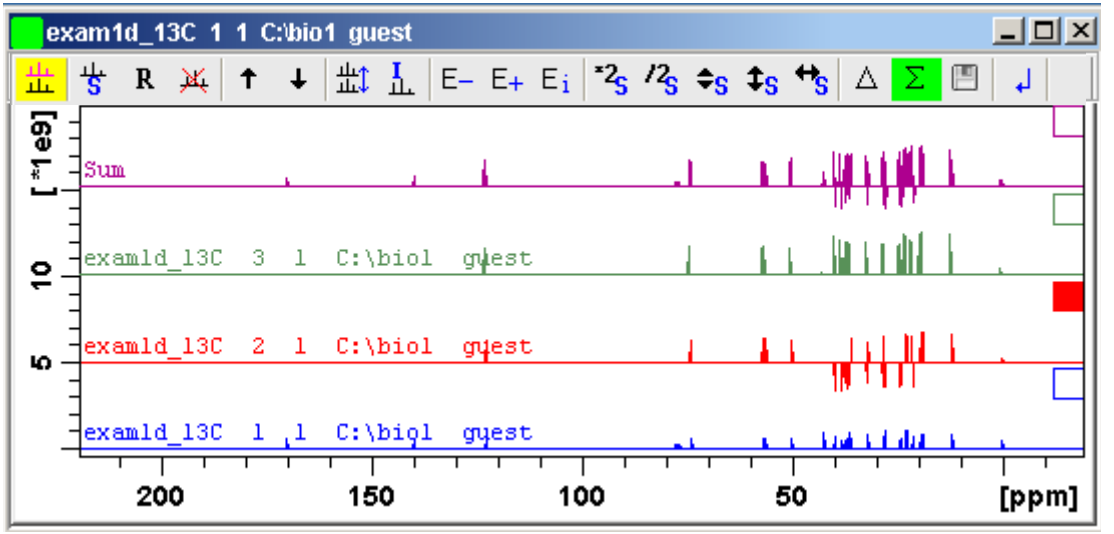


Figure 11.9 Data window in multiple display mode

The yellow button indicates that the data window is in multiple display mode.

Some buttons will turn green when they are clicked. As long as a button

is green, it is active.

Furthermore, the browser is split in two parts as shown in Fig. 11.10.

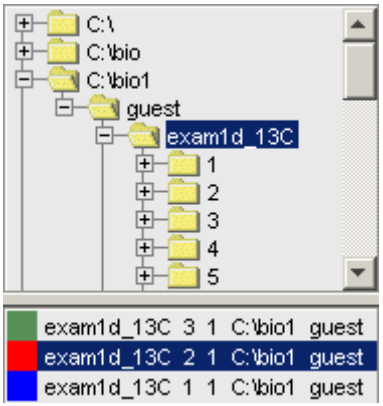


Figure 11.10

The additional lower part shows:

- which datasets are displayed in the active data window.
- which datasets are selected (these are highlighted).

How to Select/Deselect Datasets

To select a dataset:

☞ Click in the corresponding area in the data window.

or Click the small square at the upper right of the spectrum.

or Click the corresponding entry in the lower part of the browser.

In the lower part of the browser, you can:

☞ Click one dataset to select it.

or Hold down the ***Ctrl*** key and click multiple datasets to select them.

or Hold down the ***Shift*** key and click two datasets to select these two and all datasets in between.

When you select a dataset, the corresponding small square is filled (see Fig. 11.9) and its entry in the lower part of the browser is highlighted (see Fig. 11.10).

Note that:

- no spectrum selected = all spectra selected
- scale/shift buttons of the data window toolbar only work on selected spectra

To deselect a dataset:

☞ Select a different dataset.

To deselect all datasets:

☞ Click the following button:

 Deselect all datasets.

How to Remove a Dataset from Multiple Display

1. Select the dataset(s) you want to remove.
2. Click the following button:

 Remove selected data from the screen.

Note that the data on disk are not affected. Furthermore, the first spectrum cannot be removed from the screen.

How to Display the Sum or Difference Spectra

☞ Click one of the following button (button turns green):

 Show the difference between the first and the sum of the other datasets.

 Show the sum of all datasets in the multiple display window.

How to Save the Sum or Difference Spectra

1. Click the following button:

 Save the displayed sum or difference spectrum.

2. In the appearing dialog box, specify the destination *procno*.

How to Display the Next/Previous Name/Expno

To compare a series of spectra you can interactively increment or decrement the dataset name or expno. A dataset name is incremented according to the ICON-

NMR naming convention of increasing extensions, e.g. name.001, name.002 etc.

☞ Click one of the following button (button turns green):

E– Show the previous name/expno/procno of the last dataset

E+ Show the previous name/expno/procno of the last dataset

Ei Set the increment options. Clicking this button will open the following dialog:

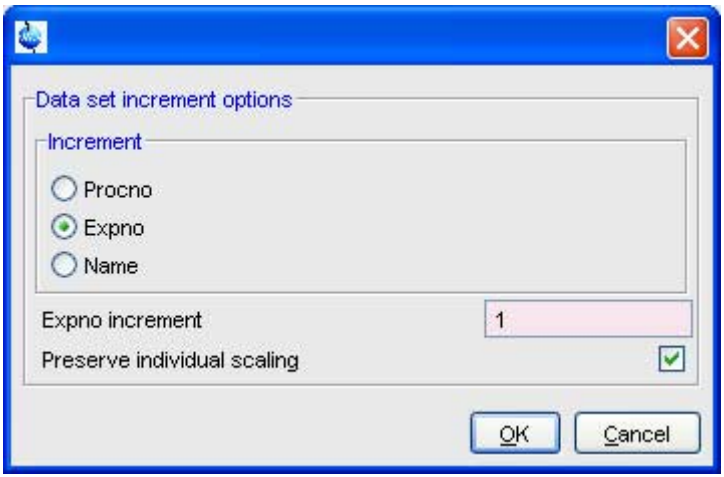


Figure 11.11

Here you can choose to increment the procno, expno or name, set the expno increment and switch individual scaling on/off.

How to Toggle between Superimposed and Stacked Display

☞ Click the following button:

Toggle between superimposed and stacked display.

How to Shift and Scale Individual Spectra

To compare the intensity and chemical shift of corresponding peaks, you can shift and scale individual spectra. To do this:

1. Display the spectra in multiple display mode as described above.
2. Expand the spectra to display the desired region or peak.
3. Select one of the spectra (e.g. by clicking it in the lower part of the browser).
4. Click-hold the button and move the mouse to align the intensities.
5. Click-hold the button and move the mouse to align the peak positions.

The alignment can be facilitated by showing the difference spectrum (button) and minimize that. Note that you can also scale the selected spectra up/down with the buttons and . The button allows you to move the selected spectra vertically. Clicking the button resets individual scaling and shifting.

The performed scaling and shifting are displayed in the data window (see Fig. 11.12 and 11.13).

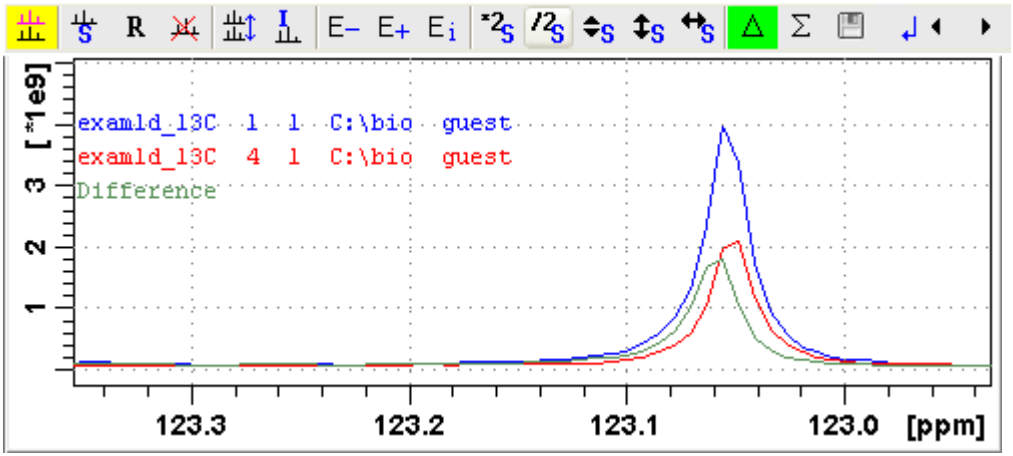


Figure 11.12

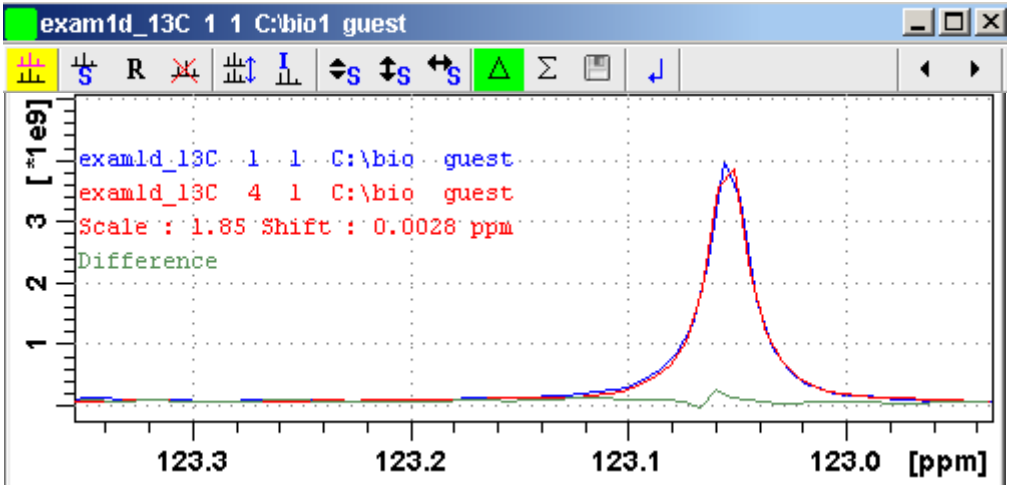


Figure 11.13

How to move the selected spectrum one place up/down

☞ Click the following button:

↑ Move the selected spectrum one place up in the list.

☞ Click the following button:

↓ Move the selected spectrum one place down in the list.

Note that the first spectrum and calculated spectra (sum of difference) cannot be moved up/down.

How to Switch on/off the Display of Datapaths and Scaling Factors

☞ Click the following button:

Switch on/off display of datapaths and scaling factors.

How to Return from Multiple Display mode

☞ Click the following button:

Return from multiple display mode [***.ret***].

How to Set the Colors of the 1st, 2nd, .. Dataset

The colors of the different datasets in the multiple display mode can be set in the *User preferences* dialog box. To set, for example, the color of the second spectrum:

☞ Click ***Options*** → ***Preferences*** and click the ***Change*** button for the item *Color of 2nd 1D spectrum*.

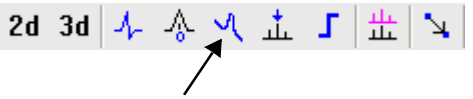
TOPSPIN 2.0 and newer allows you to set 8 different colors for different spectra in multiple display.

11.6 1D Interactive Baseline Correction

Baseline correction can be performed with commands like ***abs*** or ***absd*** or, interactively, as described below.

How to Switch to Baseline Correction Mode

☞ Click the indicated button in the upper toolbar:



or enter ***.basl*** on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig. 11.14).

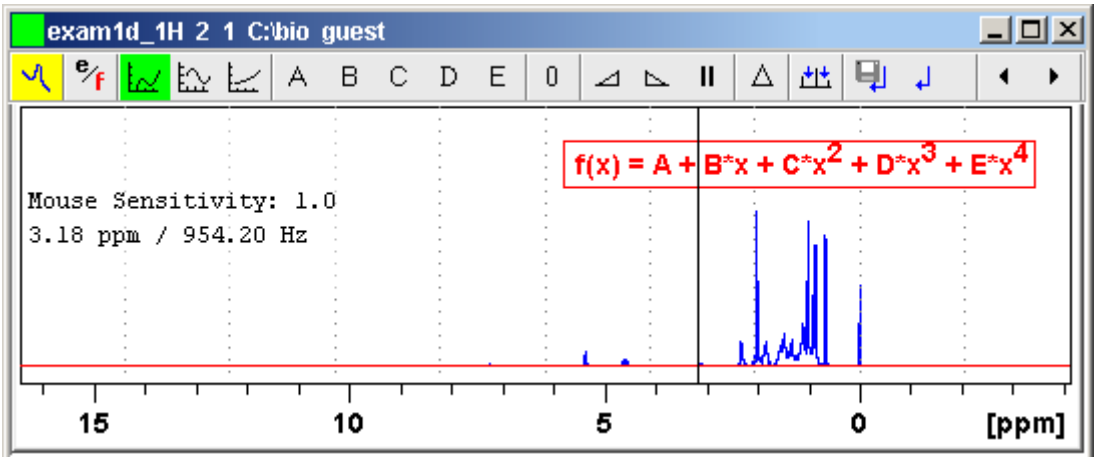


Figure 11.14 Data window in baseline correction mode

The yellow button indicates that the data window is in baseline correction mode.

Some buttons will turn green when they are clicked. As long as a button is green, it is active.

How to Perform Polynomial Baseline Correction

1. Click the following button (button turns green):

   Perform polynomial baseline correction.

   In the data window, a red horizontal line will appear as well as the equation that describes the polynomial function:

   $$f(x) = A + B*x + C*x^2 + D*x^3 + E*x^4$$

2. Click-hold button **A** and move the mouse until the red line coincides with the first point of the spectrum.
3. Repeat step 2 with the buttons **B**, **C**, **D** and **E** until the red line coincides with the entire baseline of the spectrum.

How to Perform Sine Baseline Correction

1. Click the following button (button turns green):

 Perform sine baseline correction.

A red horizontal line will appear as well as the equation describing the sine function:

$$f(x) = A + B*\sin(C*x + D)$$

2. Click-hold button **A** and move the mouse until the red line coincides with the first point of the spectrum.
3. Repeat step 2 with the buttons **B**, **C** and **D** until the red line coincides with the entire baseline of the spectrum.

How to Perform Exponential Baseline Correction

1. Click the following button (button turns green):

 Perform exponential baseline correction.

A red horizontal line will appear as well as the equation describing the exponential function:

$$f(x) = A + B*\exp(C*x)$$

2. Click-hold button **A** and move the mouse until the red line coincides with the first point of the spectrum.
3. Repeat step 2 with the buttons **B** and **C** until the red line coincides with the entire baseline of the spectrum.

How to Preview the Baseline Corrected Spectrum

Before actually performing the baseline correction, you can preview the result by displaying the difference between the uncorrected spectrum and the red correction line.

To do that:

1. Click the following button (button turns green):

 Preview corrected spectrum (show difference).

The corrected spectrum will be displayed in red.

2. If the baseline is correct, click the  button to save the correction. If further correction is needed, click the  button to show the original spectrum and the red correction line.

How to Reset the Baseline Correction Line

1. Click the following button:

   Reset the red correction line to zero.

   If the difference spectrum is displayed (the button is active), clicking the reset button will restore the original spectrum.

How to Change the Mouse Sensitivity

☞ Click one of the following buttons:

Increase (double) the Mouse Sensitivity [***.inc***].

Decrease (halve) the Mouse Sensitivity [***.dec***].

Reset the Mouse Sensitivity.

How to Save the Baseline Correction and/or Return

To return while saving the baseline correction:

☞ Click the following button:

Save baseline correction and Return [***.sret***]

This will perform the following tasks:

- Execute the baseline correction [***bcm***].
- Save the baseline correction values **A**, **B**, **C**, **D** and **E.**
- Leave the baseline correction mode.

To return while discarding any changes:

Click the following button:

Return, Discarding any changes [***.ret***].

How to Perform Cubic Spline Baseline correction

☞ Click the following button:

Define points for cubic spline baseline correction.

The toolbar of the data window will change as shown in Fig. 11.15.

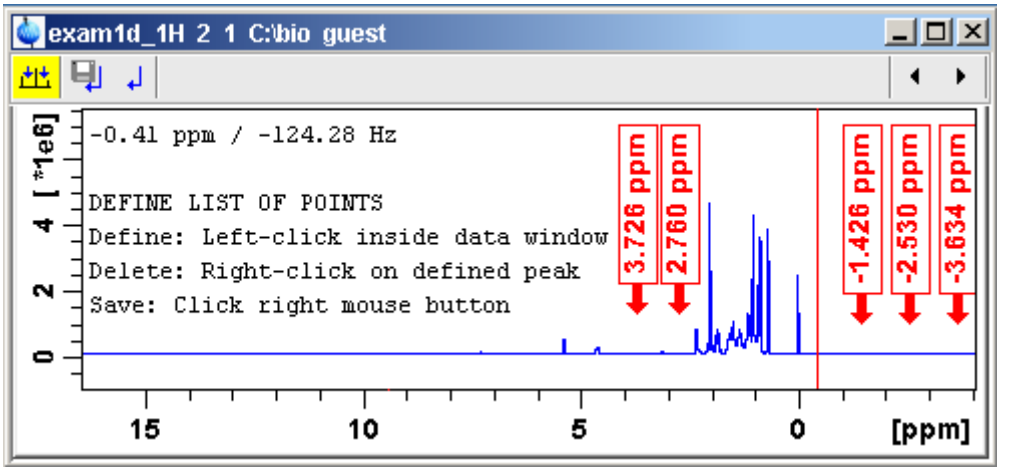


Figure 11.15 Data window in spline baseline correction mode

The cursor line in the data window turns red. If a list of baseline points already exists, you are prompted to overwrite or append to these points. If you choose ***Append***, the labels of the existing points are displayed on the screen. If you choose ***Overwrite***, no labels are displayed. Nevertheless, the existing points are only overwritten when you define and save new points.

To define new baseline points:

1. Move the cursor line to a baseline point and left-click at that position.
2. Do this for at least five baseline points.

Fig. 11.15 shows a spectrum with five defined baseline points. Note that here the points have been chosen at the right part of the spectrum for display reasons only.

How to Delete Spline Baseline Points from the screen

To delete one baseline point:

1. Right-click the baseline point position in the data window.
2. Choose ***Delete Current*** from the popup menu (see Fig. 11.16).



Figure 11.16

To delete all baseline points:

1. Right-click any position in the data window.
2. Choose ***Delete All*** from the popup menu (see Fig. 11.16).

How to Return from Cubic Spline Baseline mode with/without Save

To return while saving the baseline points:

☞ Click the following button:

Save baseline points and Return [***.retsab***].

To return while discarding any changes:

☞ Click the following button:

Return, Discarding any changes [***.ret***].

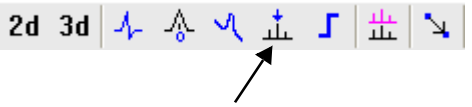
Alternatively, you can right-click in the data window and choose ***Save & Quit*** or ***Quit***, respectively.

11.7 1D Interactive Peak Picking

Peak picking can be performed, automatically, with the commands ***pps*** or, interactively, in the peak picking mode.

How to Switch to Peak Picking Mode

☞ Click the indicated button in the upper toolbar:



or enter ***.pp*** on the command line.

The Tab bar of the active data window will be replaced by a toolbar (see Fig. 11.17).

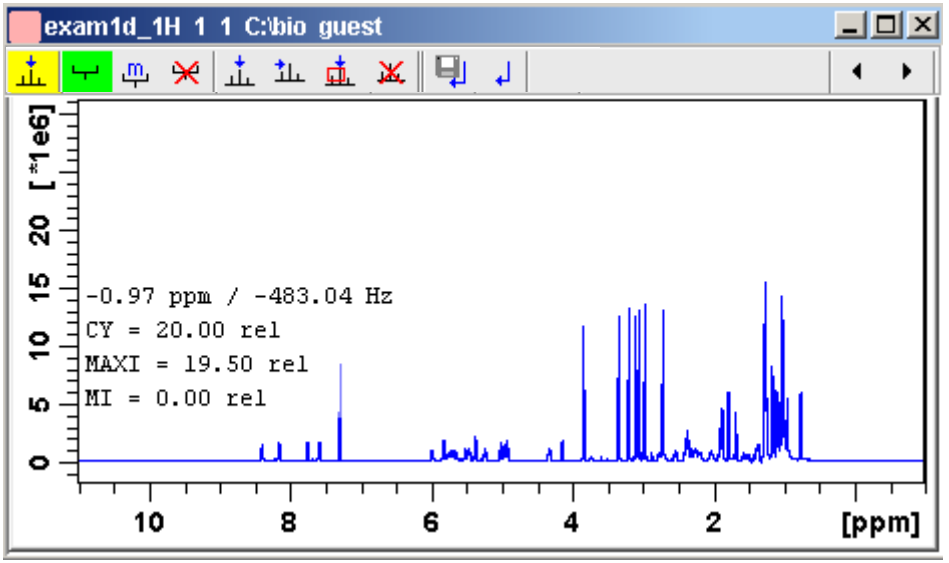


Figure 11.17 Data window in peak picking mode



The yellow button indicates that you are in peak picking mode.



Some buttons will turn green when they are clicked. As long as a button is green, it is active.

Note that the  button is automatically activated, i.e. you are in *Define peak picking range* mode

How to Define New Peak Picking Ranges

1. Put the cursor at the upper-left corner of a peak picking range.

2. Left-click-hold and drag the mouse to the lower-right corner of the range.

   The peak picking range will be marked green. The minimum and maximum intensity are set and the peaks in the range are picked and displayed.

3. Repeat step 1 and 2 for each peak picking range to be defined.
4. Click the green button to leave the "Define peak picking range" mode.

Note that the parameters MI and MAXI are set to the lowest minimum and the highest maximum intensity, respectively, of all ranges.

How to Change Peak Picking Ranges

1. Click the following button (button turns green):

    Change peak picking ranges.

2. Put the cursor on one of the edges of the peak picking range.

   The cursor turns into a double-headed arrow.

3. Left-click-hold and drag the peak range edge to its new position.
4. Optionally: repeat step 2 and 3 for the other edge and for other peak ranges.
5. Click the green button to leave the "Change peak picking range" mode.

How to Pick Peaks in Peak Picking Ranges only

Peaks in a peak range are automatically picked when the range is defined.If peaks have been deleted from a rang, they can be picked again as follows:

1. Right-click in the data field.
2. Choose ***Pick Peaks On Ranges*** from the popup menu.

Alternatively, you can enter ***ppl*** on the command line. This command can be entered in Interactive peak picking mode or in the normal display mode.

How to Delete all Peak Picking Ranges

☞ Click the  button in the data window toolbar.

or

☞ Right-click in the data field and click ***Delete All Ranges*** in the popup menu.

How to Define Peaks Manually

1. Click the following button (button turns green):

    Define peaks manually.

   A red vertical line will appear in the data window.
2. Put the red cursor line at the desired peak and click the left mouse button. The peak label will appear at the top of the data window.
3. Repeat step 2 for each peak to be defined.
4. Click the green button to leave the "Define peaks" mode.

How to Pick Peaks Semi-Automatically

1. Click the following button (button turns green):

    Define peaks semi-automatically.
2. Move the cursor into the data window.
3. Put the cursor line near the desired peak.
4. Left-click to pick forward

   or

   Right-click to pick backward (see Fig. 11.18).

   A red cursor line will appear at the nearest peak whose intensity is between MI and MAXI.
5. Right-click to add the selected peak to the peak list (see Fig. 11.18).

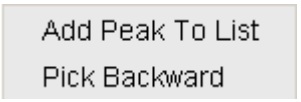


Figure 11.18

   The peak label will appear at the top of the data window.
6. Click the green button to leave the "define peaks semi-automatically" mode.

How to Delete Peaks from the Peak List

To delete a specific peak:

1. Right-click on a defined peak.

2. Choose ***Delete peak under cursor*** from the popup menu (see Fig. 11.19).

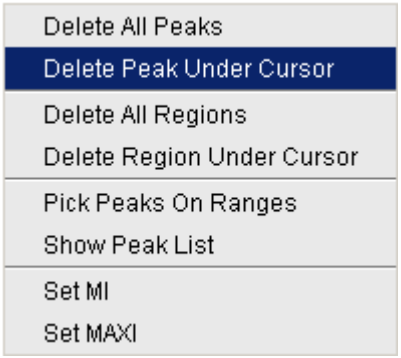


Figure 11.19

To delete all peaks:

☞ Click the button in the data window toolbar.

or

☞ Right-click in the data field and click ***Delete All Peaks*** in the popup menu.

How to Return from Peak Picking Mode with/without Save

To return while saving the peak list and peak ranges:

☞ Click the following button:

Save the Peak Region and Peak List and Return [***.sret***].

This will:

- Save the peak list to the file `peak.xml` and the peak ranges to the file `peakrng`.
- Leave the peak picking mode.

To return while discarding any changes:

☞ Click the following button:

Return, discarding any changes [***.ret***].

Chapter 12

2D Interactive Manipulation

The upper toolbar of the 2D menu offers various buttons for interactive manipulation. If you click such a button, the active data window will switch to the corresponding mode. An interactive manipulation mode is data window specific, i.e. it only applies to the active window.

12.1 2D Interactive Phase Correction

2D spectra can be phase corrected interactively in both the F2 and F1 direction by selecting certain rows and/or columns and phase correct them.

12.1.1 2D Interactive Phase Correction Procedure

How to Switch to 2D Interactive Phase Correction

Click the corresponding button in the upper toolbar as indicated below:



or enter **`.ph`** on the command line.

The Tab bar of the active data window will be replaced by a toolbar. Fig. 12.1

shows an example of an unphased 2D inverse spectrum.

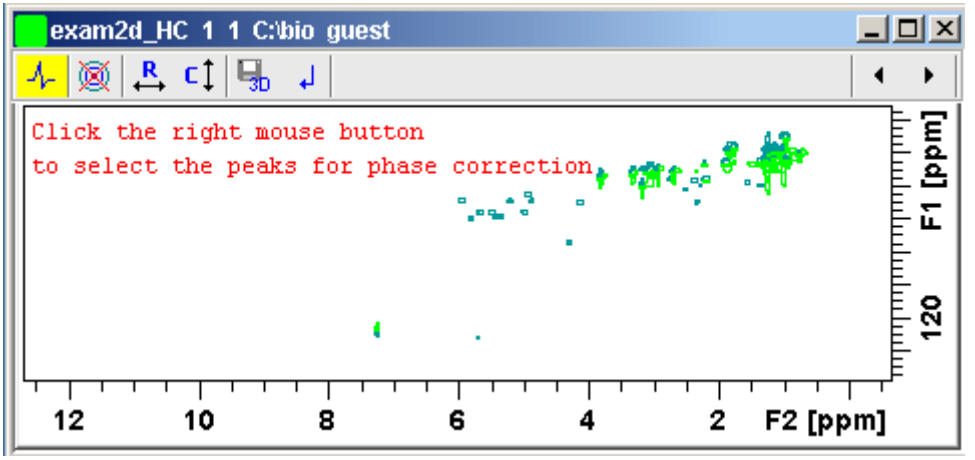


Figure 12.1 Data window in phase correction mode


The yellow button indicates that you are in phase correction mode.


Toggle the contour display on/off.


Switch to *phase row* mode to display rows of selected peaks.


Switch to *phase columns* mode to display columns of selected peaks.


Save the phase values to the 3D data from which this 2D was extracted.


Return.

How to Perform a Typical 2D Interactive Phase Correction

In this example we will perform F1 phase correction (columns) only. Take the following steps:

1. Select two or more peaks in different parts of the spectrum. To do that:
   a) Zoom in on a peak by drawing a box around it. To do that, click-hold the left mouse button and move the mouse (see Fig. 12.2).
   b) Right-click at the peak position and choose ***Add*** from the popup menu.

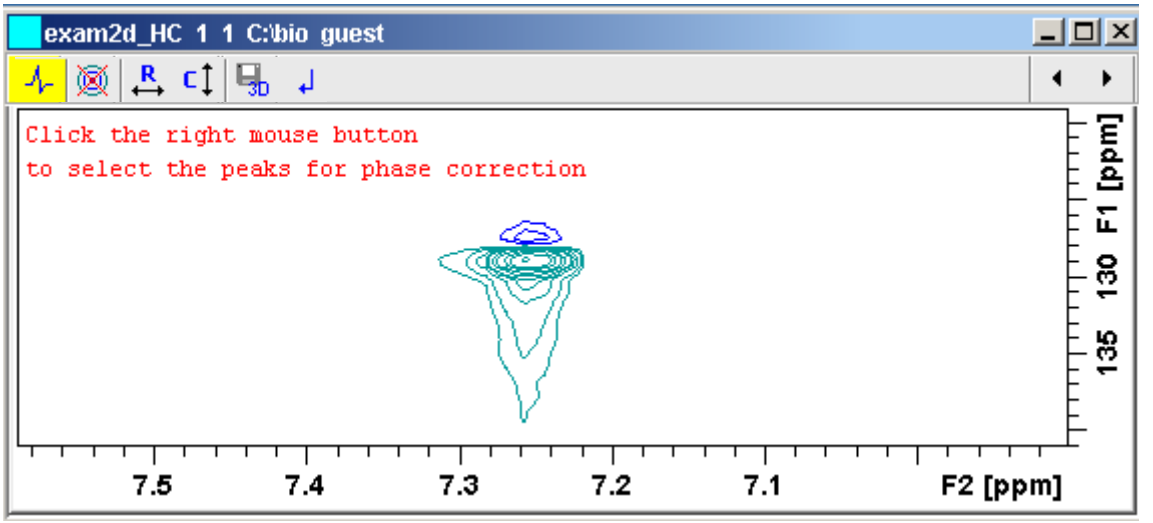


Figure 12.2

c) Click the button to display the full spectrum.

d) Zoom in on the next peak and add in the same way as the first one.

e) Zoom in on the next peak etc.

Fig. 12.3 shows an example of three selected peaks.

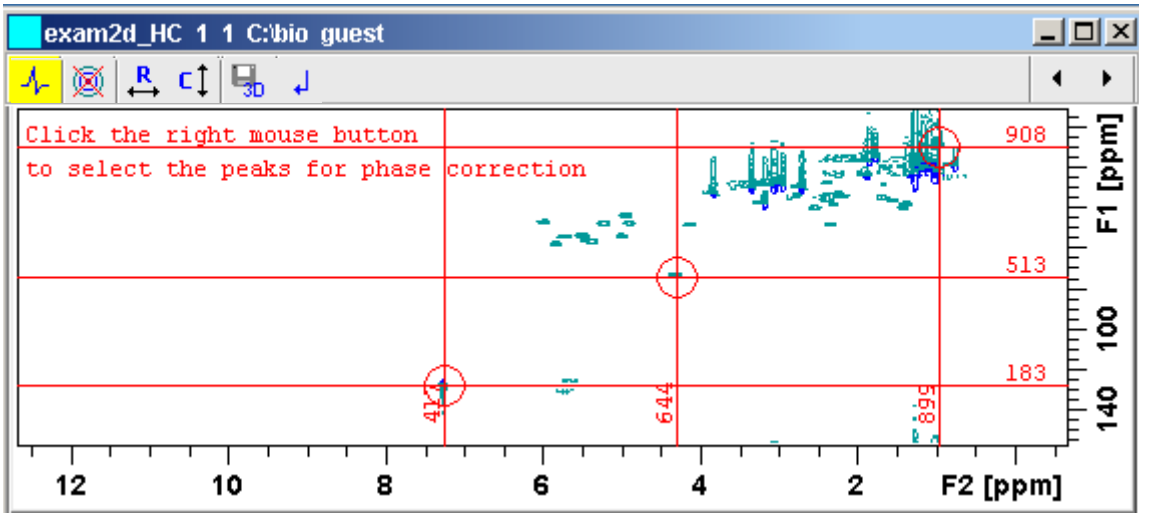


Figure 12.3

2. Click the button to phase correct the columns (F1).

   A new data window called *Phase 2D* will appear showing the columns of the selected peaks (see Fig. 12.4).

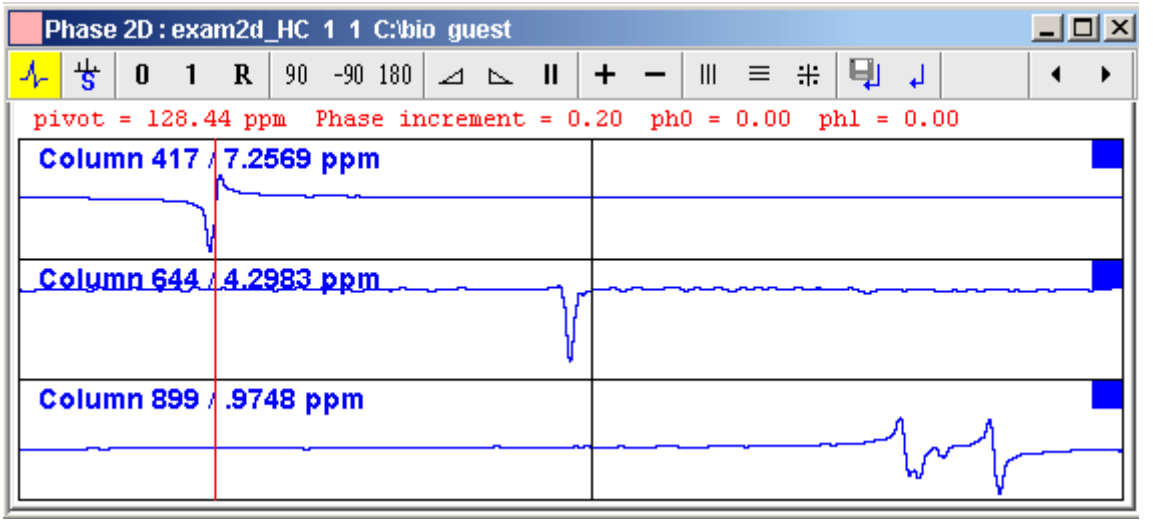

Phase 2D : exam2d_HC 1 1 C:\bio guest
0 1 R 90 -90 180
pivot = 128.44 ppm Phase increment = 0.20 ph0 = 0.00 ph1 = 0.00
Column 417 / 7.2569 ppm
Column 644 / 4.2983 ppm
Column 899 / .9748 ppm

Figure 12.4

Note that the toolbar and the right-click popup menu offer the full 1D phase correction functions.

By default, all columns are selected as indicated by the filled blue squares ■. The red vertical line indicates the default pivot point in the upper column.

3. A typical way to perform phase correction is:
   - Click-hold the 0 button for zero order correction and move the mouse until the reference peak of the first column is exactly in absorption mode.
   - Click-hold the 1 button for first order correction and move the mouse until the reference peak in other column is exactly in absorption mode.
   - Click the button to execute, save and return (see Fig. 12.5).

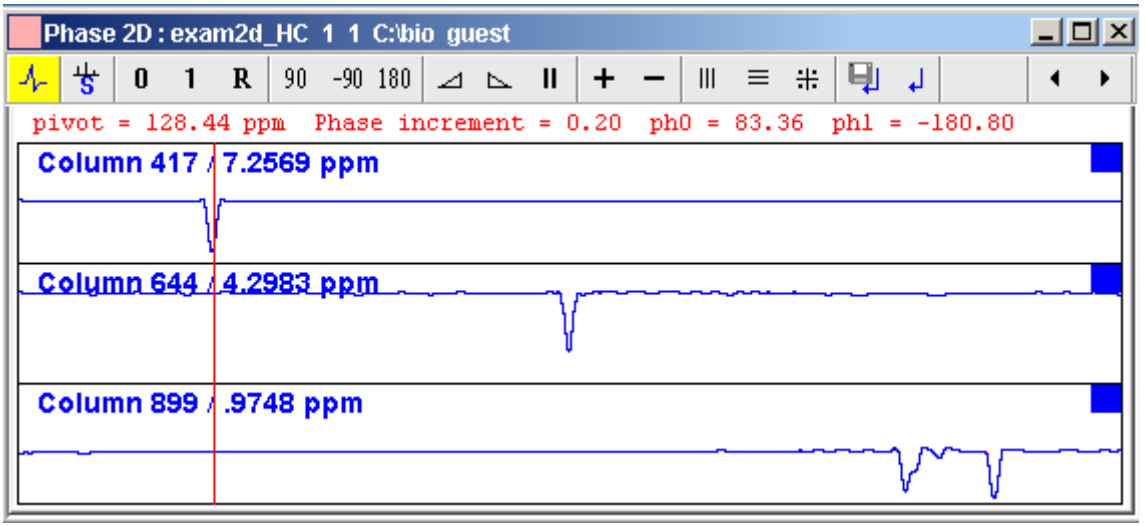

Phase 2D : exam2d_HC 1 1 C:\bio guest
0 1 R 90 -90 180
pivot = 128.44 ppm Phase increment = 0.20 ph0 = 83.36 ph1 = -180.80
Column 417 / 7.2569 ppm
Column 644 / 4.2983 ppm
Column 899 / .9748 ppm

Figure 12.5

12.1.2 2D Interactive Phase Correction Details

How to Scale or Shift Individual Rows/Columns

To select one row or column:

☞ Click in the corresponding part of the data window.

The selected row/column will be marked with a filled blue square ■ whereas unselected rows/columns will be marked with an unfilled blue square □. Selecting

a single row /column allows you to shift and scale it separately from the other rows/columns as shown in Fig. 12.6.

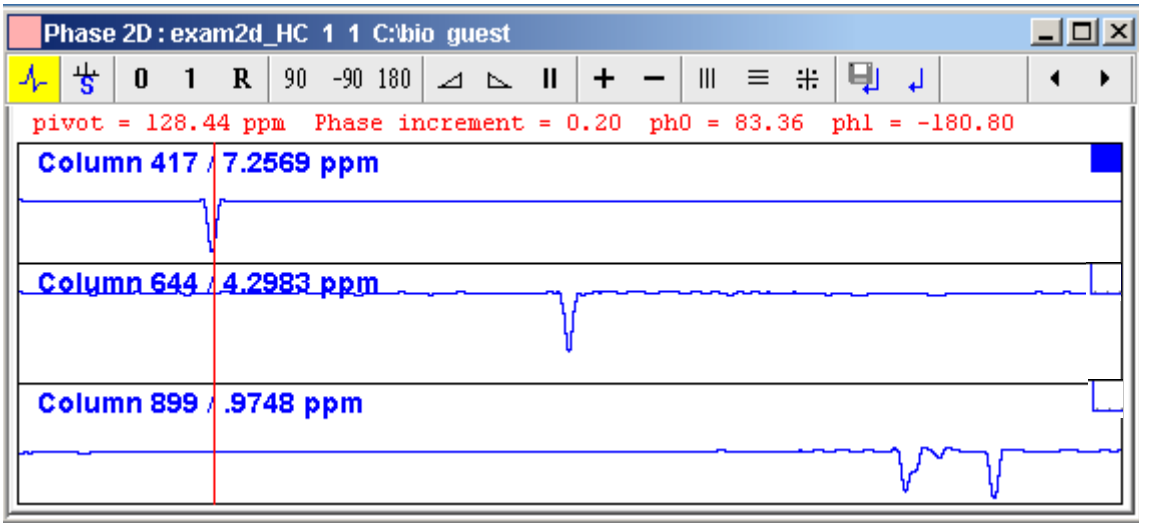

Phase 2D : exam2d_HC 1 1 C:\bio guest
0 1 R 90 -90 180
pivot = 128.44 ppm Phase increment = 0.20 ph0 = 83.36 ph1 = -180.80
Column 417 / 7.2569 ppm
Column 644 / 4.2983 ppm
Column 899 / .9748 ppm

Figure 12.6

To select all rows or columns,

☞ Click the following button:

Select all rows or columns.

How to Perform Smooth Phase Correction

To perform zero order phase correction:

1. Click-hold the following button (it turns green) and move the mouse:

   0 Zero order phase correction.

   until the reference peak of the first row/column is exactly in absorption mode.
2. Release the mouse (button turns grey).

The parameter PHC0 will be set accordingly.

To perform first order phase correction:

1. Click-hold the following button (it turns green) and move the mouse:

   1 First order phase correction.

until the reference peak of the second and further rows/columns is exactly in absorption mode.

2. Release the mouse (button turns grey).

The parameter PHC1 will be set accordingly.

How to Perform 90, -90 or 180° Zero Order Phase Correction

Click one of the following buttons:



90° zero order phase correction.



-90° zero order phase correction.



180° zero order phase correction.

How to Reset the Phase to the Original Values

Click the following button:



Reset zero and first order phase.

How to Change the Mouse Sensitivity

Click one of the following buttons:


Increase (double) the mouse sensitivity [***.inc***].


Decrease (halve) the mouse sensitivity [***.dec***].


Reset the mouse sensitivity to 1.0.

How to Show the Next/Previous Row or Column

To show the next row/column, click the following button:


Show next row/column.

Note that only the selected row/column is increased. If all rows/columns are selected, only the first one is increased.

To show the previous row/column, click the following button:

Show previous row/column.

Note that only the selected row/column is decreased. If all rows/columns are selected, only the first one is decreased.

How to Arrange Rows or Columns

Click one of the following buttons:

 Arrange rows/columns horizontally.

 Arrange rows/columns vertically (see Fig. 12.6).

 Arrange rows/columns vertically in a split window.

How to Return from Multi-1D Phase to 2D Phase Display

Click the following button:

 to save, execute and return.

This will perform the following tasks:

- Execute phase correction.
- Save the current phase correction values.
- Leave the multi-1D phase mode.

Click the following button:

 to return to the 2D phase display without save.

How to Return from 2D Phase Mode

Click the following button:

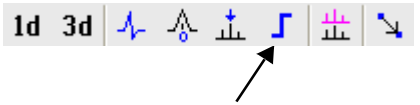
 Return.

12.2 2D Interactive Integration

TOPSPIN 2.0 and newer supports interactive 2D integration.

12.2.1 How to Switch to 2D Interactive Integration

Click the corresponding button in the upper toolbar as indicated below



or enter ***.int*** on the command line.

The Tab bar of the active data window will be replaced by a toolbar. Fig. 12.7 shows an example of a 2D inverse spectrum.

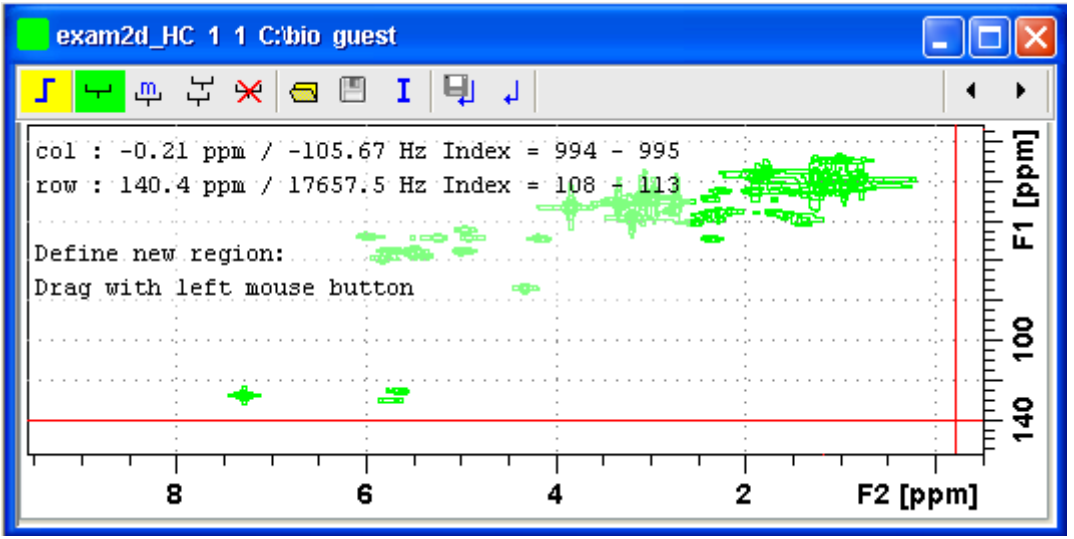


Figure 12.7 Data window in interactive integration mode

 The yellow button indicates that you are in integration mode.

 "Define integral region" mode (active when green)

 Move integral region (green when active).

 Copy a region.

 Delete all integral regions.


Read/import integral regions.


Save/Export integral regions.


Integrate current regions/define reference.


Save integral regions and return.


Return without save.

12.2.2 2D Interactive Integration Procedure

When you switch to 2D integration mode, the "Define integral region" mode is active by default. This means you can immediately start defining the integral regions. To do that:

1. Click and hold the left mouse button at any corner of a region to be defined, move the mouse to draw a box around that region and release the mouse.
2. Choose one of the following options from the appearing popup menu:

   Integrate: a : to add up all intensities in the region

   Integrate: + : to add up all positive intensities in the region

   Integrate: - : to add up all negative intensities in the region

   Integrate: a + - : to add up all intensities in the region and store separate entries for *all*, *positive* and *negative* intensities.

   Integrate: a + : to add up all intensities in the region and store separate entries for *all* and *positive* intensities.

   Integrate: a - : to add up all intensities in the region and store separate entries for *all* and *negative* intensities

   Integrate: + - : to add up all intensities in the region and store separate entries for *positive* and *negative* intensities.

   The integral regions will be displayed along with their storage numbers and

modes (see Fig. 12.8).

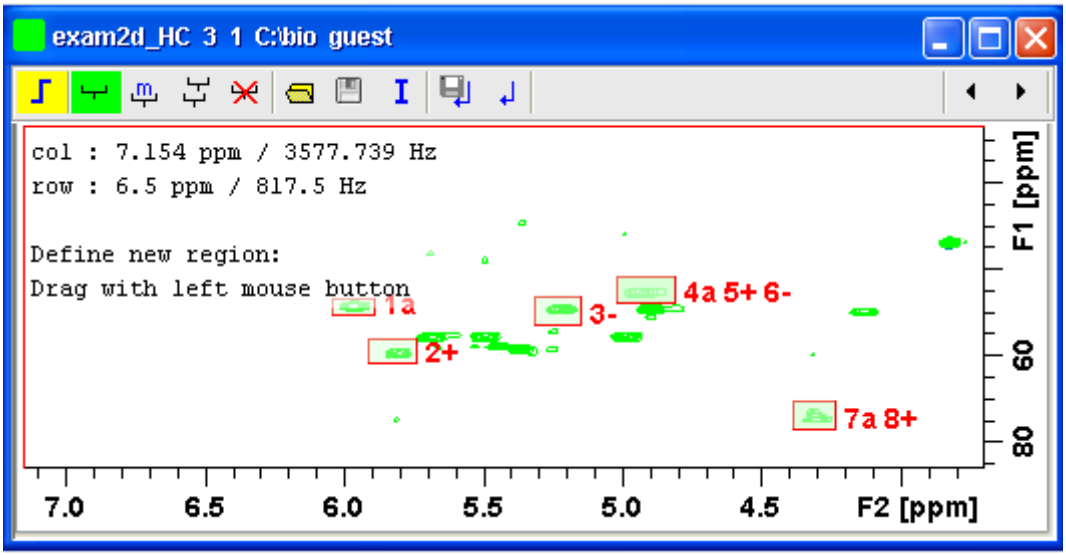


Figure 12.8

3. Click the I button and choose ***Integrate current regions*** from the pull-down menu to integrate the defined regions.
4. Click the I button again and choose ***List integral values*** from the pull-down menu to show the list of integrals.

Table 12.1 shows the list of integrals based on the regions defined in Fig. 12.8.

#	SI_F1	row1	row2	row1 ppm	row2 ppm	Abs. Int.	Integral	
	SI_F2	col1	col2	col1 ppm	col2 ppm			
1	1024	666	689	50.14583	46.43132	9.2529e+008	882.42	a
	1024	510	522	6.04420	5.89291			
2	1024	597	632	61.28934	55.71759	1.1135e+009	1062	+
	1024	520	533	5.91452	5.74162			
3	1024	652	692	52.46739	45.96701	-3.7699e+007	-35.953	-
	1024	566	579	5.31659	5.15089			
4	1024	683	721	47.35995	41.32388	1.0072e+009	960.57	a
	1024	589	605	5.02122	4.81230			
5	1024	683	721	47.35995	41.32388	1.064e+009	1014.7	+
	1024	589	605	5.02122	4.81230			
6	1024	683	721	47.35995	41.32388	-5.6725e+007	-54.097	-
	1024	589	605	5.02122	4.81230			
7	1024	502	543	76.61168	70.11130	1.2637e+009	1205.2	a
	1024	637	649	4.38726	4.23598			
8	1024	502	543	76.61168	70.11130	1.2911e+009	1231.3	+
	1024	637	649	4.38726	4.23598			

Table 12.1

Alternatively, you can define a reference integral and integrate the defined regions of the same or of a different dataset, relative to this integral. For this purpose the button offers the following menu items:

- ***Integrate current regions rel. to reference***
  You will be prompted for the reference integral number and value.
- ***List integral values***
  The output list will now show an additional column with the normalized integral values.
- ***Define current dataset as reference***
  You will be prompted for the reference integral number and value.

- ***Integrate and use ref. dataset for calibration***
  The integral value defined on the reference dataset is used for calibration.

How to Move an Integral region

1. Click the button  (it turns green).
2. Move the mouse into the region to be moved.
3. Left-click-hold and move the mouse to move the region.
4. Release the mouse at the desired position.

How to Copy an Integral region

1. Click the button  (it turns green)
2. Move the mouse into the region to be moved
3. Left-click-hold and move the mouse to the desired position
4. Release the mouse to copy the region.

How to Delete all Integral Regions

1. Click the button  .
2. Click ***OK*** to confirm deletion.

How to Read/Import Integral Regions

1. Click the button  .
2. Click ***Read intrng*** to read the last stored integral ranges

   or

   Click ***Import Integration Regions*** to import an exported integral region file (see below)

How to Save/Export Integral Regions

1. Click the button 
2. Click ***Save Regions to*** intrng to save the regions to the current dataset PROCNO (file `int2drng`)

   or

   Click ***Export Integration Regions*** to export the integration region file for general usage; i.e. usage with other datasets.

How to Return from 2D Integration mode

Click the following button:

 to save the current integral regions and return.

Click the following button:

 to return to the 2D integration mode without save.

12.3 2D Multiple Display and Row/Column Handling

2D multiple display shows a 2D spectrum with an arbitrary number of 1D and/or 2D spectra superimposed.

Spectra are ppm aligned or Hz aligned, according to the selected axis unit.

A superimposed 1D spectrum is automatically displayed in the direction of the matching nucleus (for a hetero-nuclear 2D) or in the F2 direction (for a homo-nuclear 2D).

Although multiple display is normally used for spectra with matching nuclei, it allows you to superimposed spectra with non-matching nuclei. You will get a warning that the nuclei do not match. Just just click ***OK*** to continue.

How Switch to Multiple Display mode and Read Multiple Spectra

Switching to multiple display and reading multiple spectra can be done in two different ways:

- Read a 2D dataset and click  to switch to multiple display mode. Then add 1D and/or 2D spectra, e.g. from the browser or with ***`re`***.

or

- Select multiple spectra in the browser, right-click one of them and click ***Display***.

For a more detailed description of reading multiple data in multiple display mode, see chapter 11.5.

In multiple display mode, the Tab bar of the active data window is replaced by

a toolbar (see Fig. 12.9).

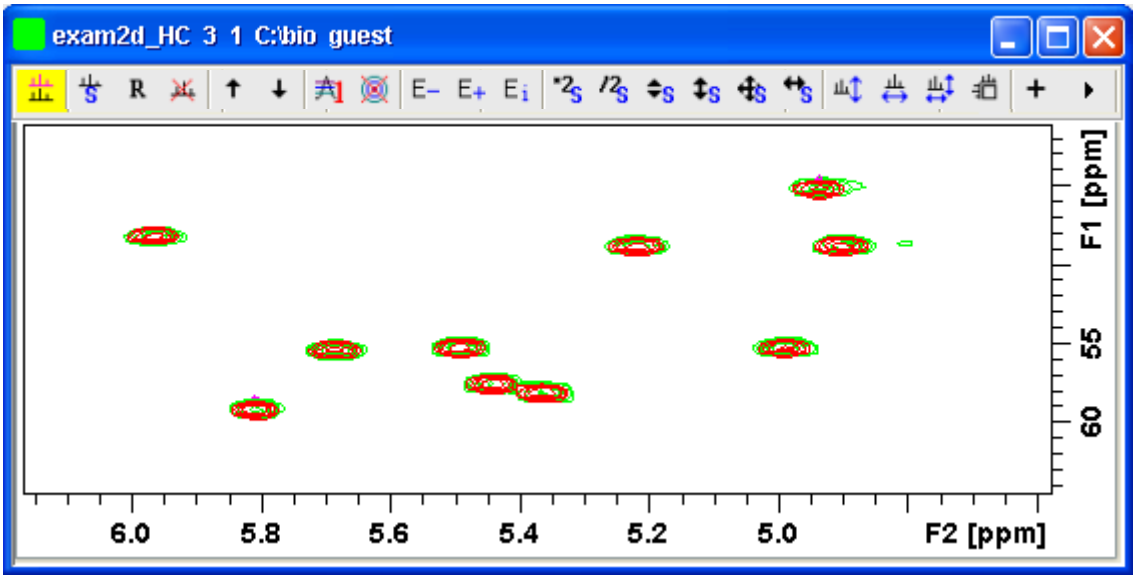


Figure 12.9 Multiple display with two 2D spectra superimposed

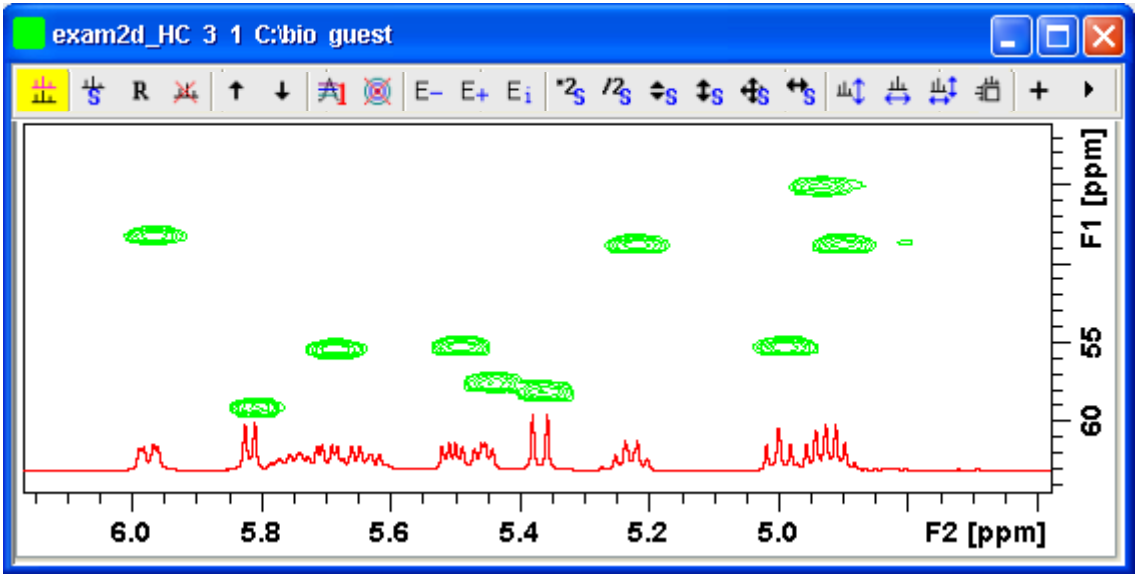


Figure 12.10 Multiple display with a 1D spectrum superimposed on a 2D spectrum



The yellow button indicates that the data window is in multiple display mode.



Some buttons will turn green when they are clicked. As long as a button is green, it is active.

The browser in multiple display is split in two parts (see Fig. 12.11).The additional lower part shows:

- which datasets are displayed in the active data window
- which datasets are selected (they are highlighted)

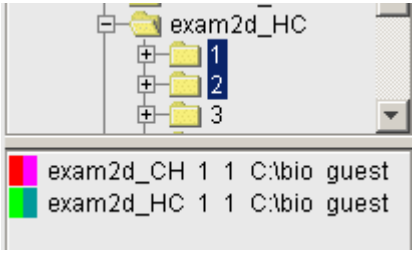


Figure 12.11

How to Align Multiple 2D Spectra

2D spectra in multiple display can be individually shifted. To do that:

1. Select one of the spectra in the lower part of the browser.
2. Click-hold the  button and move the mouse.

Fig. 12.12 shows a region of two comparable 1H/13C inverse 2D datasets which are shifted relative to each other.

Clicking the  button resets individual scaling and shifting.

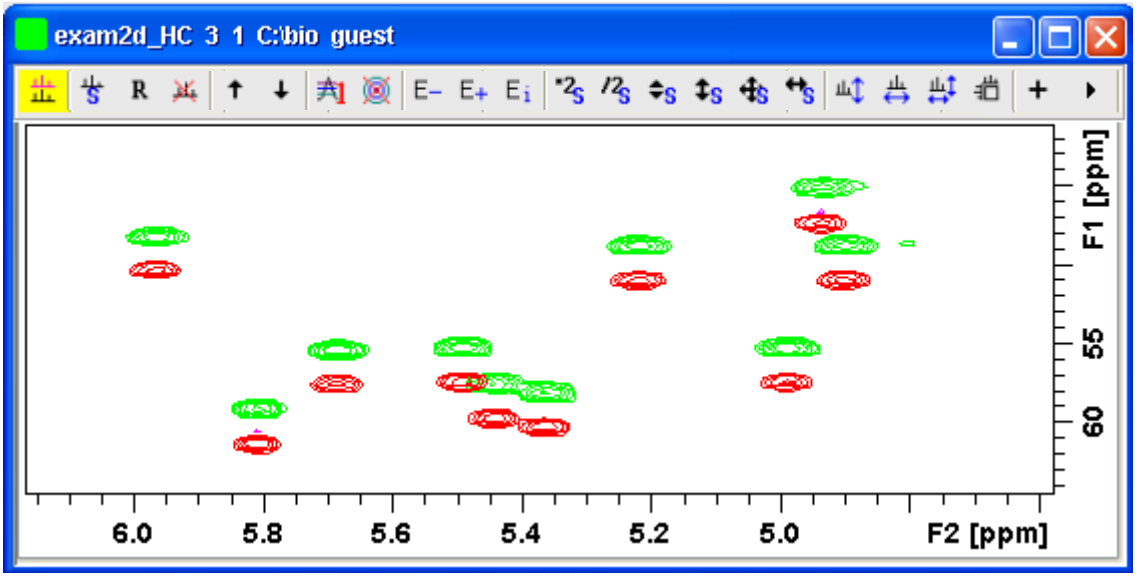


Figure 12.12

How to Display the Next/Previous Name/Expno

To compare a series of spectra you can interactively increment or decrement the dataset name or expno. A dataset name is incremented according to the ICON-NMR naming convention of increasing extensions, e.g. name.001, name.002 etc.

☞ Click one of the following button (button turns green):

E– Show the previous name/expno/procno of the last dataset

E+ Show the previous name/expno/procno of the last dataset

Ei Set the increment options. Clicking this button will open the following dialog where you can choose to increment the procno, expno or name, set the expno increment and switch individual scaling on/off.

How to Scan Rows/Columns

Click the following button (it turns green) and move the mouse in the data field:

to scan rows in the 2D spectrum.

Click the following button (it turns green) and move the mouse in the data field:

 to scan columns in the 2D spectrum.

Click the following button (it turns green) and move the mouse in the data field:

 to scan rows and columns in the 2D spectrum.

To scale up the displayed row/column:

☞ Click the left mouse button or turn the mouse wheel up.

To scale down the displayed row/column:

☞ Click the middle mouse button or turn the mouse wheel down.

How to Grab a Row/Column

You can grab a row or column, i.e. keep it displayed in the data window as follows:

1. Scan rows or columns as described above and hold at the desired position.
2. Right-click in the data window.
3. Choose ***Grab Row/Column*** from the popup menu (see Fig. 12.13).

Note that a grabbed row/column appears in the lower apart of the browser. It can be selected there and individually scaled or shifted.

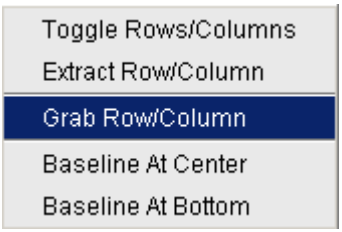


Figure 12.13

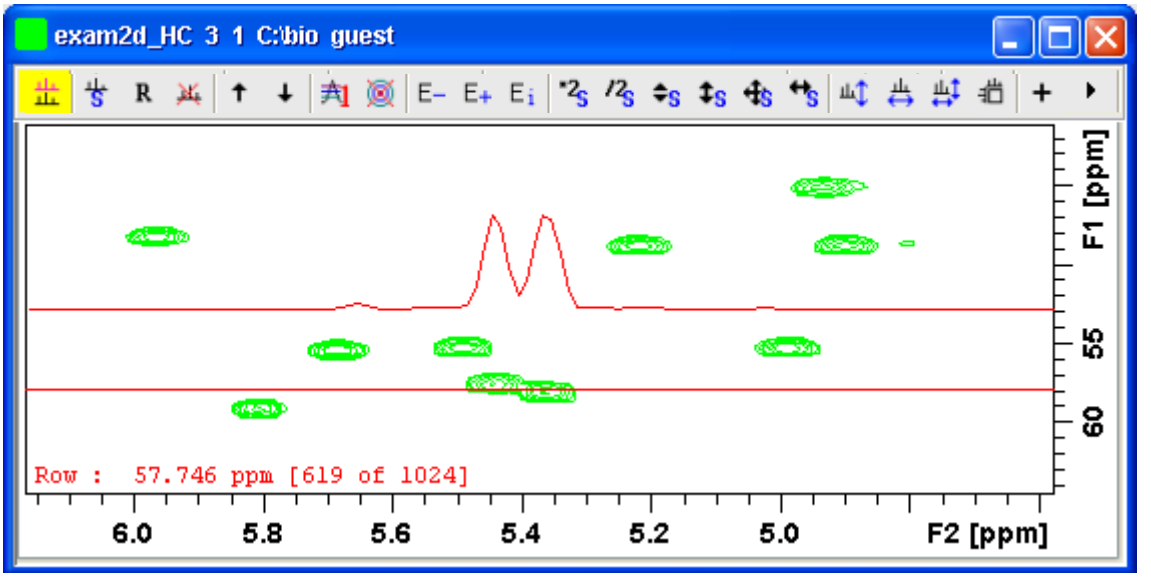


Figure 12.14

Fig. 12.14 shows row 619 with the 1D baseline at the center of the data window.

How to Show the Next/Previous Row or Column

To show the next row/column, click the following button:

+ Show next row/column.

To show the previous row/column, click the following button:

− Show previous row/column.

Alternatively, you can turn the mouse wheel, while pressing the Shift key to show the next/previous rows/columns.

How to Move the Selected Dataset Up/Down in the Dataset List

To move the selected dataset up, click the following button:

↑ Move the selected dataset up.

To move the selected dataset down, click the following button:

↓ Move the selected dataset down.

How to Extract a Row/Column

1. Scan rows or columns as described above and hold at the desired position.
2. Right-click in the data window and choose ***Extract Row/Column*** from the popup menu (see Fig. 12.13).
3. Specify the row/column number and output *procno* in the dialog box. Note that the ROW/COLUMN field is initialized with the grabbed row/column or, if no grabbing was done, with the current row/column.
4. Click ***OK***

The extracted row or column is stored as a 1D dataset under the specified PROCNO and displayed in a new data window. In the upper left part is this, the row number and source 2D dataset is specified (see Fig. 12.15).

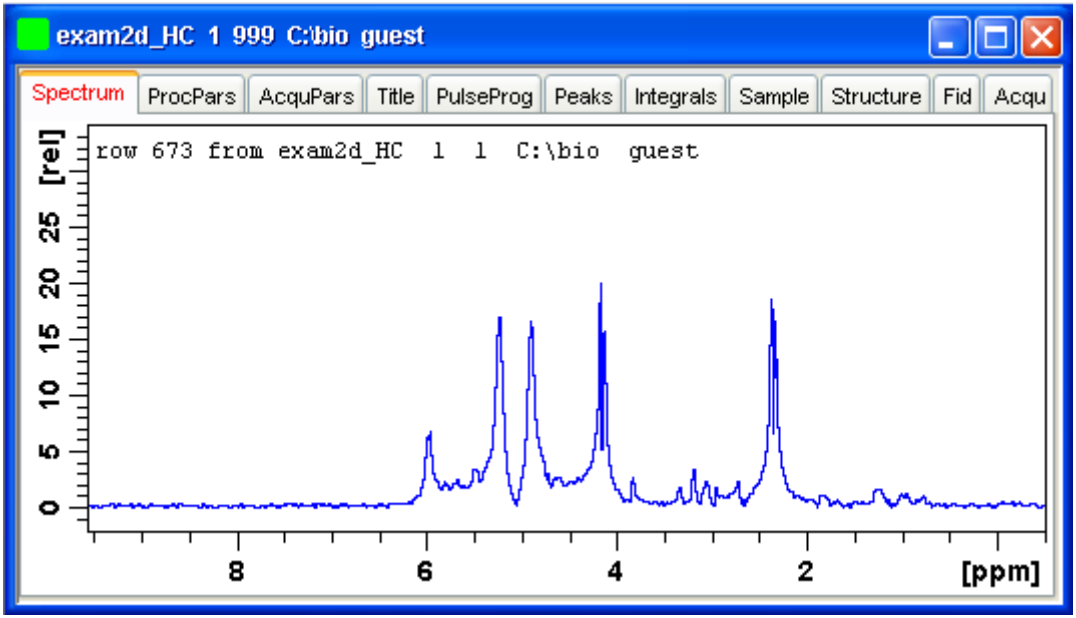


Figure 12.15

How to Copy Contour Levels from First to Other Spectra

Click the following button:

Copy contour levels from the first to the other spectra.

Note that the contour levels are only changed on screen, not on disk.

How to Switch on/off 2D contour display

Click the following button:

 Switch on/off 2D contour display.

How to Position the Baseline of the Row/Column

To put the baseline at the center of the data window:

1. Right-click in the data window.
2. Choose in ***Baseline At Center*** from the popup menu (see Fig. 12.13).

To put the baseline at the bottom of the data window:

1. Right-click in the data window.
2. Choose in ***Baseline At Bottom*** from the popup menu (see Fig. 12.13).

This works both in the scan submode or on a grabbed row/column.

12.4 2D Interactive Calibration

A 2D spectrum can be calibrated, automatically with the command ***sref*** or, interactively as described below.

How to Switch to 2D Calibration mode

☞ Click the corresponding button in the upper toolbar:.



or enter ***.cal*** on the command line. The Tab bar of the active data window will be replaced by a toolbar (see Fig. 12.16).

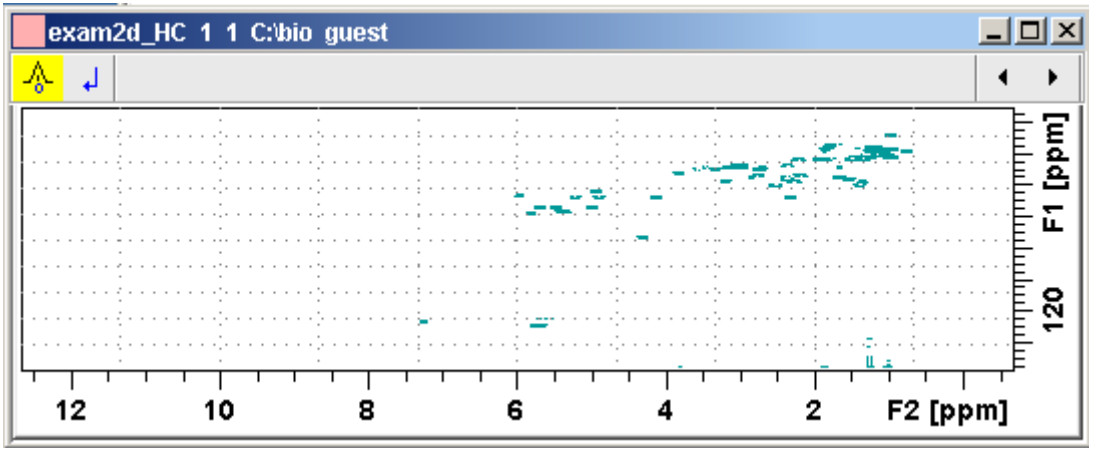


Figure 12.16 Data window in calibration mode

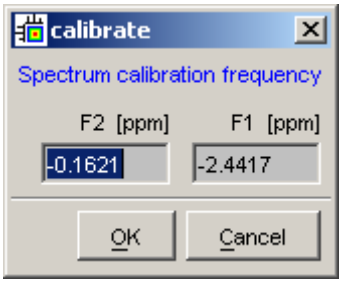
The yellow button indicates that the data window is in calibration mode.

How to Perform 2D Calibration

In calibration mode:

1. Left-click in the data window at the reference peak.

   The following dialog box will appear:



   Note that the units for F2 and F1 (Hz or ppm) correspond to the axis units of the display.

2. Enter the F2 and F1 frequency you want to assign to the reference peak.
3. Click ***OK***.

The spectrum will be calibrated and re-displayed. The calibration button will turn grey again.

12.5 2D Chemical Shift Distance Measurement

How to Measure a 2D Chemical Shift Distance

1. Click the following button (button turns green):

   Chemical shift distance measurement.

2. Click-hold the left mouse button at one peak position and drag the mouse to another peak position.

   The distance in ppm, will be displayed.

3. Right-click in the data window to quit distance mode (button turns grey).

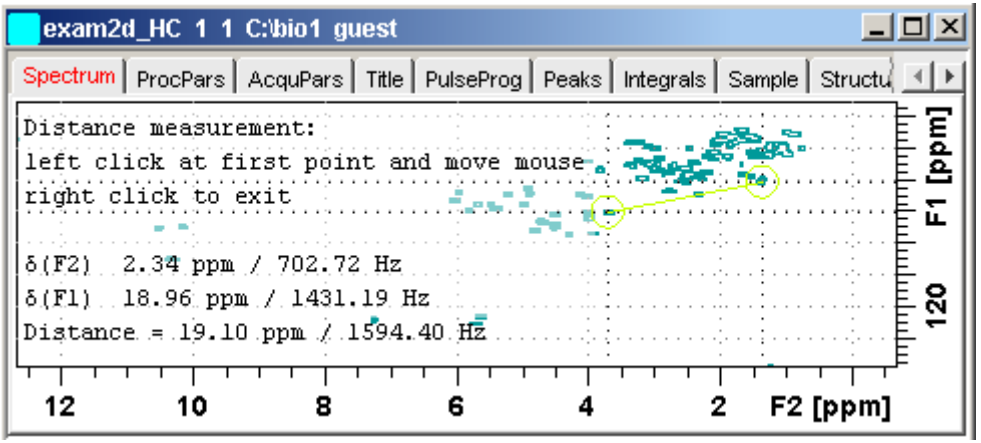


Figure 12.17 Data window in distance measurement mode

Chapter 13

Data Window Handling

13.1 Data Windows

The TOPSPIN window has a data area that may contain multiple data windows. The size of the data area depends on the overall size of the TOPSPIN window and on presence of the Browser and/or Processing Guide. Fig. 13.1 shows the TOPSPIN window with the Browser and three data windows.

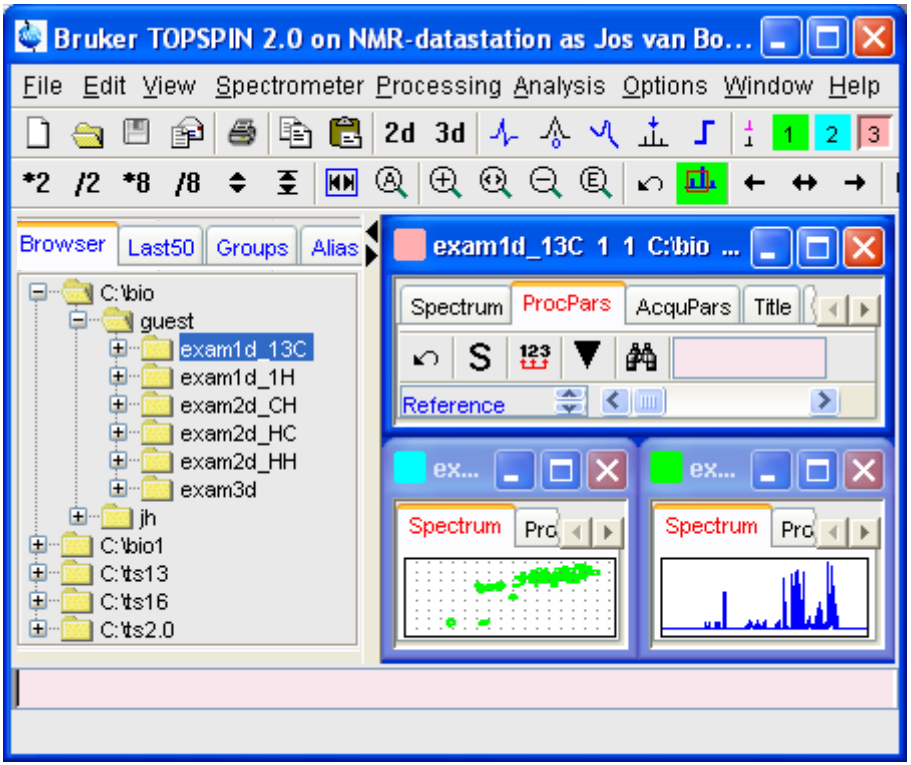


Figure 13.1

Note that the three data windows show different data objects: 1D processing parameters, a 1D spectrum and a 2D spectrum.

How to Move a Data Window

☞ Click-hold the title bar and move the mouse.

How to Resize a Data Window

1. Move the cursor to the window edge until it becomes a double-headed arrow.
2. Left-click-hold that position and move the mouse.

Depending on the position of the double-headed arrow, you can change the window height, width or both (see Fig. 13.2)

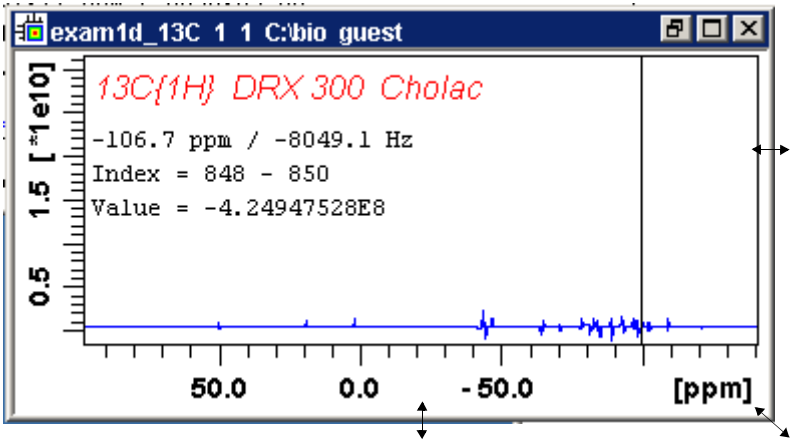


Figure 13.2

How to Select (activate) a Data Window

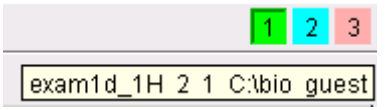
The active data window is the window of which the title bar is highlighted. The TOPSPIN menu, tool bars and command line commands correspond to and act on that window. Only one data window is active at a time.

To activate a different data window:

☞ Click in the desired data window or click its title bar.

or

☞ Click one of the colored radio buttons above the data area. The pressed radio button (the green one in the example below) corresponds to the current dataset.



If you hold the cursor over one of the buttons without clicking it and wait a few seconds, the corresponding dataset specification will be shown.

or

☞ Click ***Window*** → ***x dataname expno procno dir user***

where ***x*** is the number of the desired window and ***dataname***, ***expno***, ***procno, dir*** and ***user*** refer to the dataset displayed in that window.

or

☞ Hit the ***F6*** key to activate the next window. Repeat that until the desired window is the active window.

How to Open a New empty Data Window

☞ Click ***Window*** → ***New window [Alt+w-n]***

The new data window will become the active window and will, by default, cover the entire data area, hiding possible existing data windows. To open a dataset in the new window, drag a dataset from the browser or from the Windows Explorer into the new window or click ***File*** → ***Open*** (see also chapter 4.3).

How to Arrange Data Windows

If the data area contains multiple data windows, you can arrange them in various ways. All the arrange commands arrange the windows left to right and/or top to bottom in the order in which the windows have been active. The currently active data window will therefore be positioned at the top and/or left of the data area.

To arrange the data windows as a grid:

☞ Click ***Window*** → ***Arrange as a Grid***

Depending on the number of windows, they will be arranged vertically and/or horizontally (see Fig. 13.3).

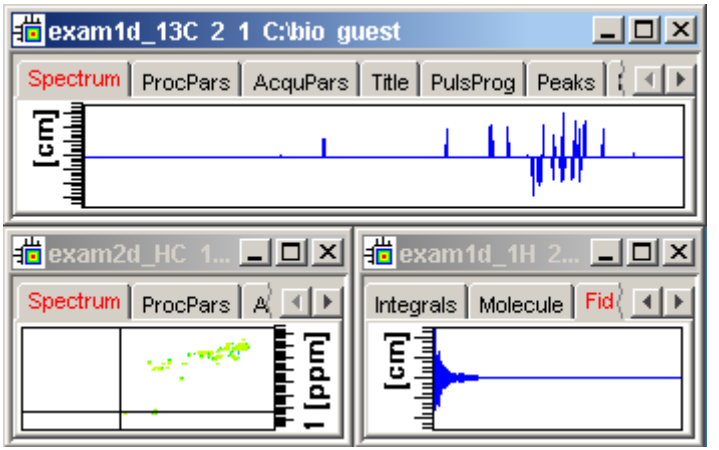


Figure 13.3

To arrange data windows in stack (see Fig. 13.4):

☞ Click ***Window*** → ***Arrange in Stack***

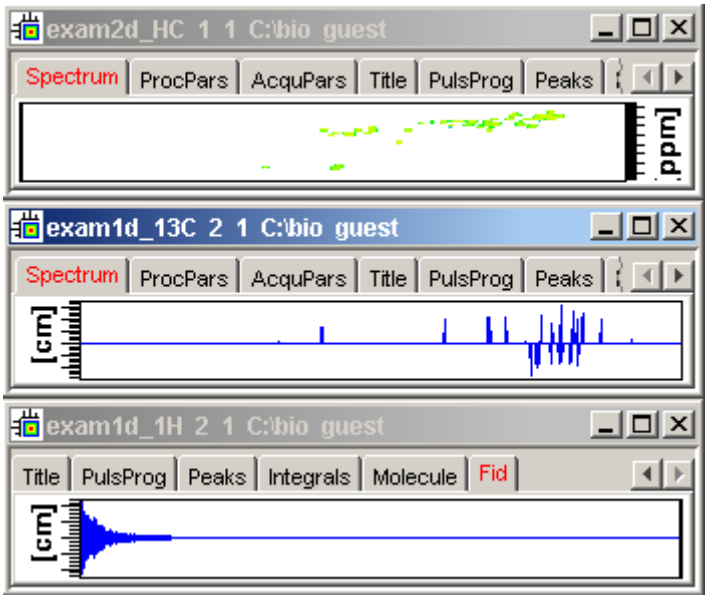


Figure 13.4

To arrange data windows side by side (see Fig. 13.5):

☞ Click ***Window*** → ***Arrange Side-by-Side***

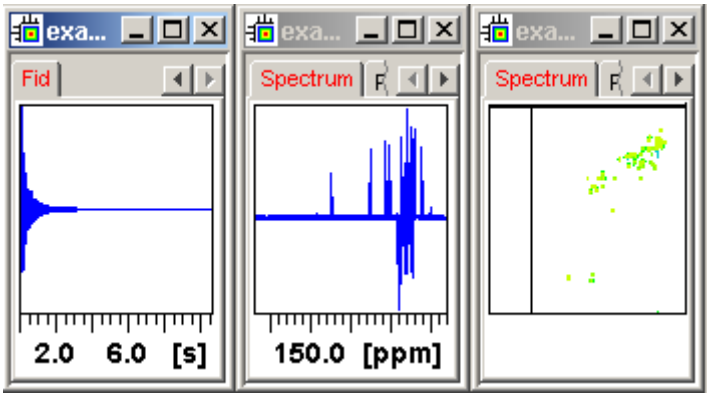


Figure 13.5

To cascade data windows (see Fig. 13.6):

☞ Click ***Window*** → ***Cascade***

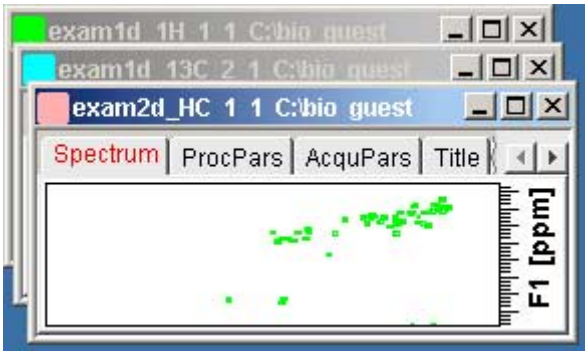


Figure 13.6

Note that you can instruct TOPSPIN to open new data windows cascaded rather than maximized as well configure cascaded windows (command ***`set`*** → ***Window settings***, see also chapter 4.3)

How to Iconify (minimize) a Data Window

☞ Click the button in the windows title bar

or

☞ Click ***Window*** → ***Iconify all*** to iconify all windows.

How to De-iconify a Data Window

☞ Click the button or double-click the title bar.

How to Maximize a Data Window

☞ Click the button or double-click the title bar.

The window will cover the entire data area. Note that a maximized window cannot be moved of resized but can be restored (in size and position), iconified or closed.

How to Restore the Size and Position of a Data Window

☞ Click the button or double-click the title bar.

Note that this is only possible if the title bar contains the button. This is only the case after the window has been maximized or iconified.

How to Close a Data Window

To close the active data window:

☞ Click ***File*** → ***Close*** [`Crtl-w`]

or

☞ Click the button in the windows title bar.

To close any data window:

☞ Click the button in the data windows title bar

or

☞ Click the title bar and then click ***File*** → ***Close*** [`Crtl-w`].

To close all data windows:

☞ Click ***File*** → ***Closeall*** [`closeall`]

How to Iconify all Data Windows

☞ Click ***Window*** → ***Iconify all***

How to Maximize all Data Windows

☞ Click ***Window*** → ***Maximize all***

The active window will be displayed on top, all other windows are hidden.

How to Activate the Next Data Window

☞ Click ***Window*** → ***Next window*** [***F6***].

The windows title bar will become highlighted.

13.2 Window Layouts

A data window layout defines the position, geometry and window type of one or more TOPSPIN windows. The following windows types are available:

- data windows
- lock display window
- acquisition display window
- BSMS display window
- temperature unit window

How to Save the Current Window Layout

1. Click ***Window*** → ***Save layout***
2. In the appearing dialog box:
   Specify the layout File name (extension `.prop`) and click ***Save Layout***

How to Read a Window Layout

1. Click ***Window*** → ***Read layout***
2. In the appearing dialog box:
   Specify or click the layout File name and click ***Read Layout***

Windows are arranged according to the following rules:

- Each currently displayed window type gets the position and geometry to the corresponding definition in the layout.
- If a window type is displayed but not defined in the layout, it keeps its current position and geometry.
- If a window type is defined in the layout but not displayed, the layout definition is ignored.
- Multiple *data* windows are, arbitrarily, assigned to the available data window definitions.

How to Swap Data Windows

Within a certain layout, you can easily swap two TOPSPIN windows with the command ***swin***. If the data area contains exactly two windows, ***swin*** simple swaps their position and geometry. If it contains more than two data windows, ***swin*** opens a list from which you can select any window to be swapped with the currently selected (active) window. Swapping windows can also be executed from the ***Window*** menu.

Chapter 14

Analysis

14.1 Introduction

TOPSPIN offers various data analysis methods including chemical shift measurement, signal to noise calculation and T1/T2 relaxation analysis as described in this chapter. Furthermore, it offers the following structure analysis tools:

- Multiplet Analysis
  This allows you to easily define multiplets and deduce chemical shifts, coupling constants, multiplicities and connections.
- Daisy (TOPSPIN 2.0 and newer)
  This allows you to simulate spectra based on chemical shifts and coupling constants.
- Solids Line Shape Analysis
  This allows you to simulate and fit calculated spectra to various experimental 1D solid NMR spectra.
- Jmol
  A 3D Structure Viewer for displaying chemical structures.
- 2D molecule structure editor
  A program for drawing chemical structures., offering a large number of drawing tools.

- DNMR (Dynamic NMR) Lineshape Analysis
  A program to simulate temperature dependent NMR spectra, interactively set up and iteratively refine the model parameters to get the best fit of the measured and simulated 1D NMR spectra.

Structure analysis tools can be started from the ***Analysis*** menu. They are all described in the following manuals:

☞ Click ***Help*** → ***Manuals*** → [**Analysis and Simulation**] ***Structure Analysis Tools***

except for Daisy, which is described in the separate manual:

☞ Click ***Help*** → ***Manuals*** → [**Analysis and Simulation**] ***Daisy***

14.2 1D Chemical Shift Distance Measurement

How to Measure a Chemical Shift Distance

1. Click the following button (button turns green):

    Chemical shift distance measurement.

2. Left-click-hold at one peak position and drag the mouse to another peak position.

   The distance in ppm, will be displayed.

3. Right-click in the data window or move the cursor out of the data window to leave distance measurement mode (button turns grey).

14.3 1D Signal to Noise Calculation

How to Perform Interactive S/N Calculation

1. Click ***Analysis*** → ***Signal/Noise Calculation*** [`.sino`].

   The current signal region (parameters SIGF1-SIGF2) and noise region (parameters NOISF1-NOISF2) are displayed.

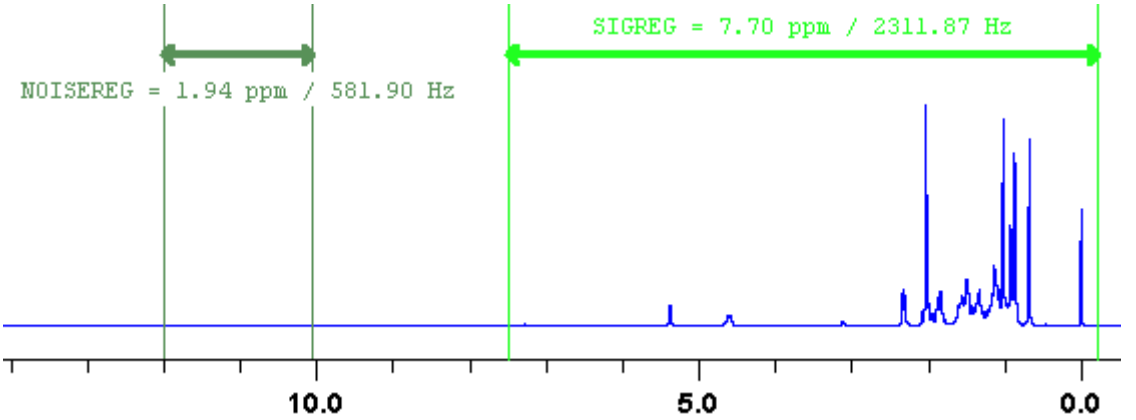


Figure 14.1 Data window in S/N measurement mode

2. Move the mouse into the data window.
3. Left-click-hold and drag the mouse from one edge of the *signal* region to the other edge.

   A horizontal double-headed arrow will indicate the signal region.
4. Left-click-hold and drag the mouse from one edge of the *noise* region to the other edge.

   A horizontal double-headed arrow will indicate the noise region.
5. Right-click any position in the data window. The popup menu as shown in Fig. 14.2 will appear.

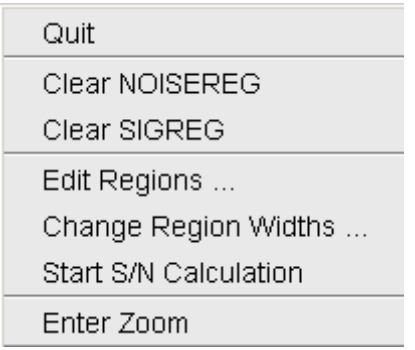


Figure 14.2

Choose ***Start S/N calculation***

The other entries allow you to redefine or clear the regions. After the noise calculation has finished, the result will appear on the screen.

How to Delete the Signal Region or Noise Region

To delete the current signal region:

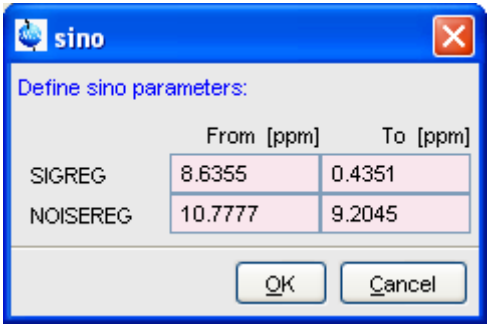
1. Right-click in the data window.
2. Choose ***Clear SIGREG*** from the popup menu (see Fig. 14.2).

To delete the current noise region:

1. Right-click in the data window.
2. Choose ***Clear NOISEREG*** from the popup menu (see Fig. 14.2).

How to Edit the Limits of the Signal Region or Noise Region

1. Right-click in the data window.
2. Choose ***Edit regions...*** from the popup menu (see Fig. 14.2).
3. Enter new limit values in the appearing dialog box.



4. Click ***OK***

The S/N value is automatically recalculated and displayed.

How to Change the Width of the Signal Region or Noise Region

1. Right-click in the data window.
2. Choose ***Change region width...*** from the popup menu (see Fig. 14.2).

3. Enter new width values in the appearing dialog box.



4. Click ***OK***

Note that as you change the width, the right limit is modified correspondingly. The left limit is kept. The S/N value is automatically recalculated and displayed.

14.4 Relaxation Analysis

Typically, relaxation data consist of a series of 1D FIDs measured with varying delays and stored as pseudo 2D data. To analyze these data, Topspin offers an easy to use T1/T2 Relaxation Guide. Relaxation curves of various experiment types with up to six components can be fitted.

To start the Relaxation Guide:

☞ Click ***Analysis*** → ***T1/T2 Relaxation*** [**`t1guide`**].

This will open the dialog box as shown in Fig. 14.3.

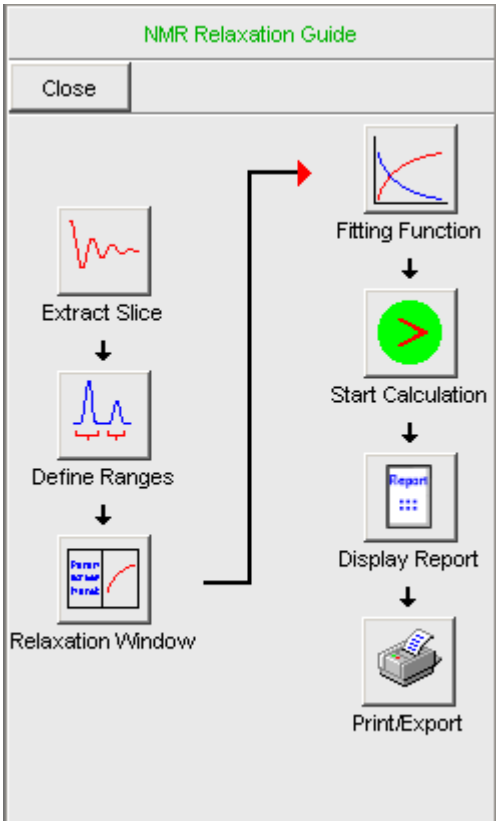


Figure 14.3

Just click the successive icons and follow the instructions on the screen. Note that holding the cursor over an icon shows the command line command that is executed when the icon is clicked. If you prefer to execute these commands from the command line, just click the ***Close*** button to close the Relaxation Guide.

Extract Slice

Prompts you for the FID or spectrum to be extracted for peak determination (see Fig. 14.4). Click ***FID*** to extract an FID or ***Spectrum*** to extract a spectrum. Note that the latter only works if the pseudo 2D data have been processed. If you click

FID, the extracted FID is automatically processed. We recommend to enter the

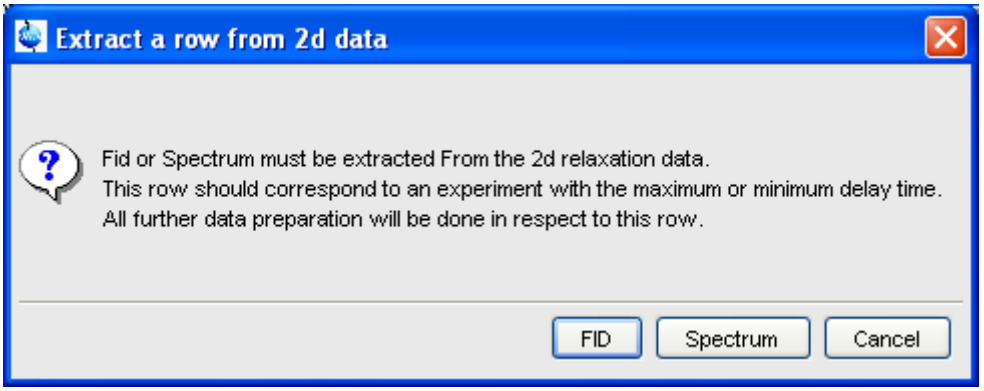

Extract a row from 2d data
Fid or Spectrum must be extracted From the 2d relaxation data.
This row should correspond to an experiment with the maximum or minimum delay time.
All further data preparation will be done in respect to this row.
FID
Spectrum
Cancel

Figure 14.4

FID or spectrum number which was measured with the longest delay. It can be found in the *vdlist* file in the EXPNO data directory. Then you can choose between:

- ***Manual Integration***. This will switch to Interactive integration mode The highest peak in each region will be used for relaxation analysis.
- ***Manual Peak Picking***. The selected peaks will be used for relaxation analysis.

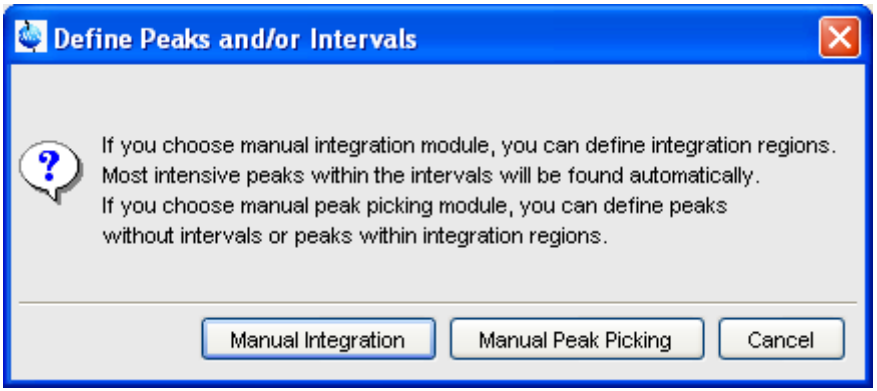

Define Peaks and/or Intervals
If you choose manual integration module, you can define integration regions.
Most intensive peaks within the intervals will be found automatically.
If you choose manual peak picking module, you can define peaks
without intervals or peaks within integration regions.
Manual Integration
Manual Peak Picking
Cancel

Figure 14.5

Peaks/Ranges

Switches to interactive integration or peak picking mode as chosen above. Here

you can define the ranges or peaks to be included in the relaxation analysis. Then use button to export regions/peaks to Relaxation Module and quit the interactive mode.

Relaxation Window

Switches the 1D data window to relaxation analysis mode (see Fig. 14.6)

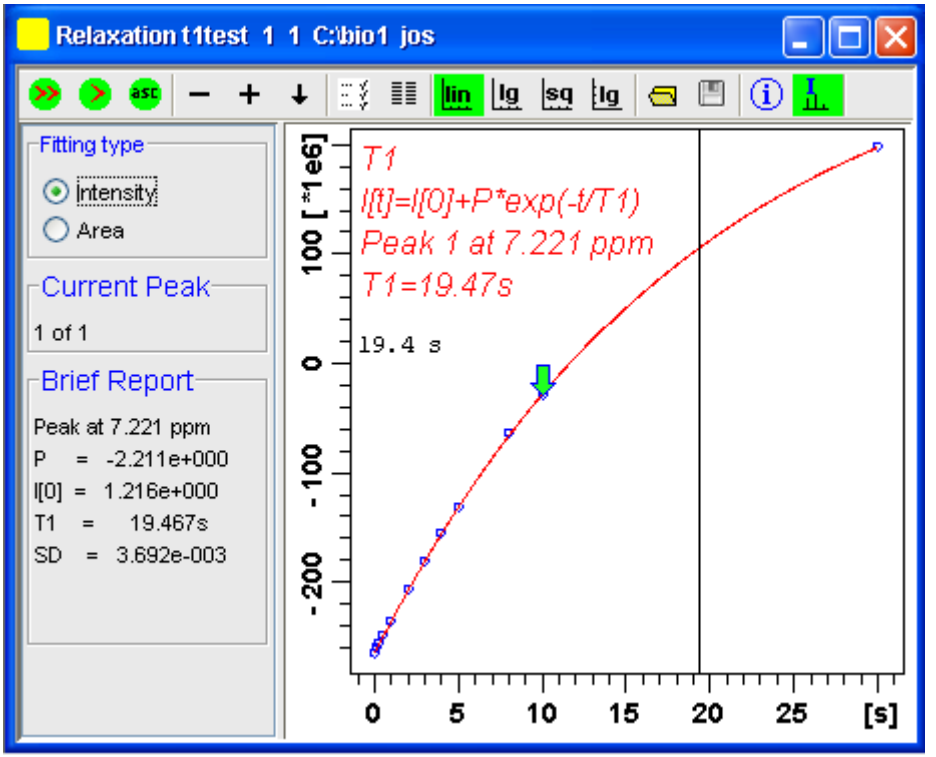


Figure 14.6

and performs a default fitting. By default, this is one-component, T1-intensity fitting (Function type *uxnmrt1*) for peak 1. If the dataset was already fitted, the previous type of fitting is performed. The fitting curve is displayed in the data section and a *Brief Report* is shown in the parameter section. If this default fitting is appropriate, you can view, interpret and print the results as described below. If not, you can perform the desired fitting as described below.

Perform Fitting and Calculate the Relaxation Time

Depending on the experiment, you can perform the appropriate fitting as follows:

1. Select a ***Fitting type***: *Intensity* or *Area*. Either every point reflects the intensity of the biggest peak in the defined integral range or the integral itself. Both of them can be used but, depending on the experiment, one of them usually give a better fitting curve.
2. Click the button to open the parameter dialog box. Select a ***Function Type*** and set the required parameters (see below).
3. Click ***OK***.
4. Perform fitting and calculate the relaxation time:

   Fit the relaxation curve for the current peak.

   Fit the relaxation curve for all peaks.

   Fit data according to the ASCII file t1ascii.

View and interpret the results as described below.

Function Types and Parameters

The TOPSPIN relaxation routine offers functions for various relaxation experiments with up to 6 components:

uxnmrt1 for one-component T1 experiments. Set the parameter *List file name* to the list type used during the acquisition. Set ***Pick data points*** to PD or PD0 (see below). The T1 fitting function is defined by the function:

$$I(t) = I(0) + P \times \exp\left(\frac{t}{T1}\right)$$

where *I* is Intensity or Area according to the Fitting Type. The best fit is calculated by varying I(0), P and T1 in an iterative process according to the Levenberg-Marquardt algorithm. Clicking and executes the commands ***ct1*** (current peak) and ***dat1*** (all peaks), respectively.

uxnmrt2 for one-component T2 experiments. Set the parameter *List file name* to the list type used during the acquisition. Set ***Pick data points*** to PD or PD0 (see below). A T2 fitting function is defined by the function:

$$I(t) = P \times \exp\left(\frac{t}{T2}\right)$$

where *I* is Intensity or Area according to the Fitting Type. The best fit is calculated by varying P and T2 in an iterative process according to the Levenberg-Marquardt algorithm. Clicking  and  executes the commands ***ct2*** (current peak) and ***dat2*** (all peaks), respectively.

invrec, satrec, cpt1rho, expdec, gaussdec, lorgauss linear, varbigdel, varlitdel, vargrad, vardamp: these functions can be used for various experiments with up to 6 components, except for **cpt1rho** and **lorgauss** which allow only 4 and 3 components, respectively. They all use the simplex algorithm and require some parameters to be set:

- Enter the **Number of components**
- Click the ***Setup*** button to set the *Iteration Control parameters*. For each component, the initial guess (G) and step rate (S) can be set. The initial guess for I[0] must be selected such that the sum of all components does not exceed 1. If there is only one component, I[0] is usually set to 1.The step rate is usually set to about one tenth of the initial guess. If the step rate of a variable is set to zero, then this variable is not changed during the iterations. Note that the initial guesses can also be set with the  toolbar button. Clicking  and  executes the commands ***simfit*** (current peak) and ***simfit all*** (all peaks), respectively.

The Fitting Function to pick data points can be:

- ***pd*** - pick data points for relaxation analysis (Drift value interpreted)
- ***pd0*** - pick data points for relaxation analysis at constant peak positions (drift value ignored)

- ***pft2*** - pick data points for T2 calculation of 1D raw data.

View the Fitting Results

When the fitting procedure has finished, the fitting curve is displayed in the data section and a *Brief Report* appears in the parameter section (see Fig. 14.6). The latter consists of:

- the calculated relaxation value
- the fitted parameters
- the standard deviation SD

For further examination of the result, click one of the following buttons:

Show the fitting result of the previous peak/area.


Show the fitting result of the next peak/area.



Switch x-axis to linear scaling.



Switch x-axis to logarithmic scaling.



Switch x-axis to square root scaling.



Switch y-axis to logarithmic scaling. Note that this only works for curves with positive intensities/areas only.


Import integrals from dataset ~TEMP.


Export integrals to dataset ~TEMP


Toggle button to hide/show information in the curve field, including algorithm, peak number and relaxation value.


Show an extended report, including the fitted intensity or area distribution. This consists of the same information as the brief report plus a table with the intensity or area distribution. Example:

```
Dataset : C:/bio/data/guest/nmr/t1test/1/pdata/1

INTENSITY fit :

 I[t]=I[0]+P*exp(-t/T1)
```

```
12 points for Peak 1,  Cursor Point =  7.221 ppm

Results     Comp. 1


I[0]  =   1.215e+000
P     =   -2.211e+000
T1    =      19.449s
SD    =   3.685e-003

    tau    ppm     integral    intensity

30.000s    7.221  2.5811e+009  1.9737e+008
10.000s    7.221 -3.2898e+008 -2.9056e+007
8.000s     7.221 -7.8525e+008 -6.4616e+007
5.000s     7.221 -1.6289e+009 -1.3101e+008

...
```

Print, Export of Copy the Fitting Results

To print the fitting curve:

☞ Click ***File*** → ***Print***

To export the fitting curve as a graphics file:

☞ Click ***File*** → ***Export***

To copy the fitting curve to the Windows Clipboard:

☞ Click ***Edit*** → ***Copy***

Chapter 15

Acquisition

This chapter describes TOPSPIN acquisition as far as the interface is concerned. Individual acquisition command are described in the Acquisition Reference manual.

15.1 Acquisition Guide

If you are a new or occasional user, we recommend you to acquire your data with the TOPSPIN Acquisition Guide. This will guide you through the typical sequence of acquisition steps. To start the Acquisition Guide, click ***Spectrometer → Acquisition Guide***.

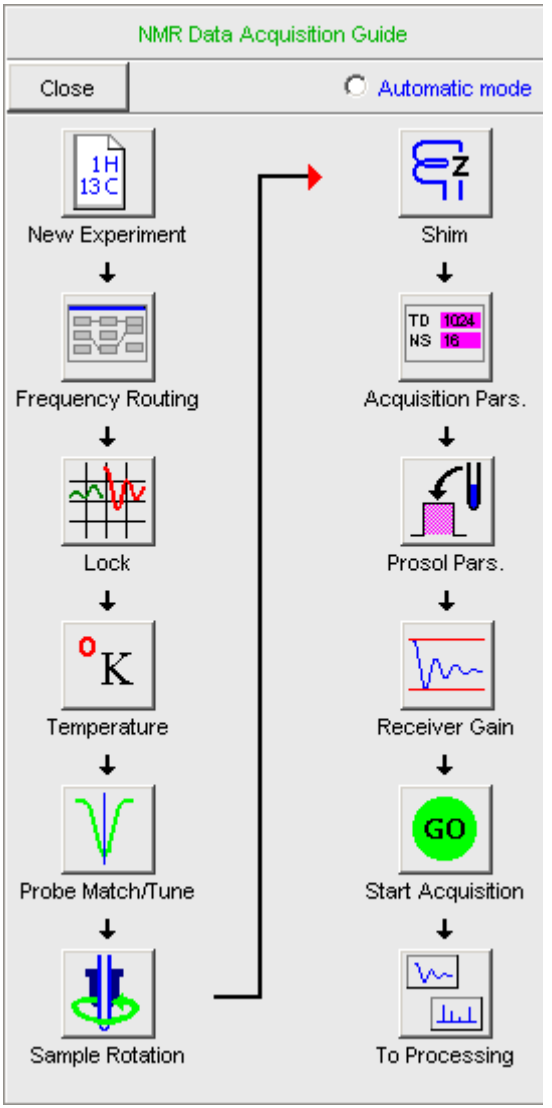


Figure 15.1

In ***Automatic mode***, the Acquisition Guide will simply execute each command when you click the respective button. This requires the acquisition parameters to be set correctly. In interactive mode (***Automatic mode*** unchecked), the Acquisition Guide will, at each step, open a dialog box offering you the available options and

required parameters. Note that the last button ***To processing*** will open the processing equivalent of the Acquisition Guide, the Processing Guide.

15.2 Acquisition Toolbar

Acquisition can be prepared, started and controlled from ***Spectrometer*** menu. Clicking this menu opens the pulldown menu shown in Fig. 15.2 :

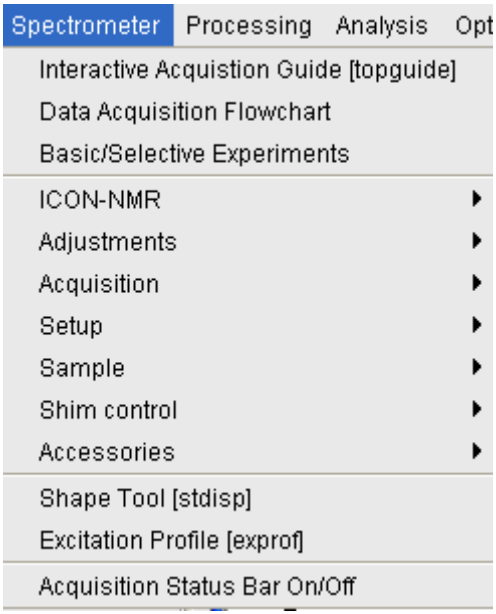


Figure 15.2

Here you find several cathegories of acquisition related commands. Each entry give access to a submenu with various commands. Fig. 15.3, for example, shows the ***Setup*** submenu.

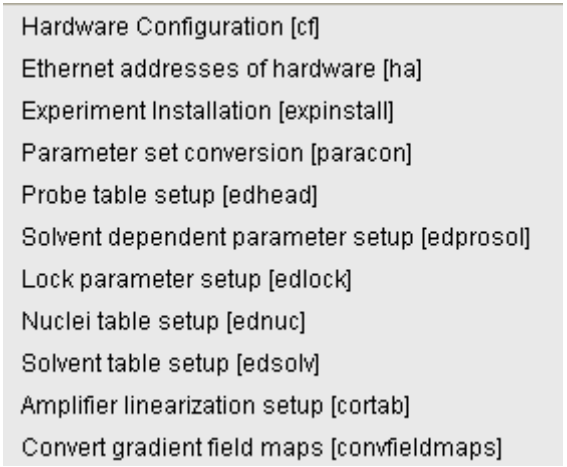

Hardware Configuration [cf]
Ethernet addresses of hardware [ha]
Experiment Installation [expinstall]
Parameter set conversion [paracon]
Probe table setup [edhead]
Solvent dependent parameter setup [edprosol]
Lock parameter setup [edlock]
Nuclei table setup [ednuc]
Solvent table setup [edsolv]
Amplifier linearization setup [cortab]
Convert gradient field maps [convfieldmaps]

Figure 15.3

For most entries, the command line command, for example ***expinstall***, is specified in square brackets. Furthermore, Topspin can be configured such that right-clicking any menu entry will display the corresponding command line command. To do that right-click in an empty part of the menubar and choose ***Define Right-click Action***.

For convenience, common acquisition commands can also be started from the TOPSPIN toolbar. The right part of the upper toolbar shows the following buttons:



- Start the acquisition. Acquires NS scans in the current dataset, overwriting possibly existing data. Equivalent to the command ***zg***.
- Halt the acquisition. This stops the acquisition after the current scan has finished. All data acquired so far are saved. Equivalent to the command ***halt***.
- Stop the acquisition. This stops the acquisition immediately. Data acquired after the last disk write (if any) are lost. Equivalent to the command ***stop***.
- Open the online FID display window. Shows the currently acquired FID. Only works during acquisition. Equivalent to the command ***acqu***.
- Open the Lock display window. Shows the lock signal. Equivalent to the command ***lockdisp***.

Calculate the experiment time. Shows the total experiment time and file size of the raw data. Equivalent to the command ***expt***.

Set SFO1, O1, O2 and O3 interactively. Puts a red cursor line in the data window. A left-click at the desired frequency opens a dialog box where you can set O1, O2 and/or O3.

Set the sweep width to the current region and the spectrometer frequency to the center of the current region. Update the parameters SW and SFO1, respectively.

Setup a frequency list interactively.

15.3 Data window Toolbar

TOPSPIN 2.0 and newer support dataset specific acquisition the display. It is activated by clicking the ***Acqu*** tab of the data window toolbar.

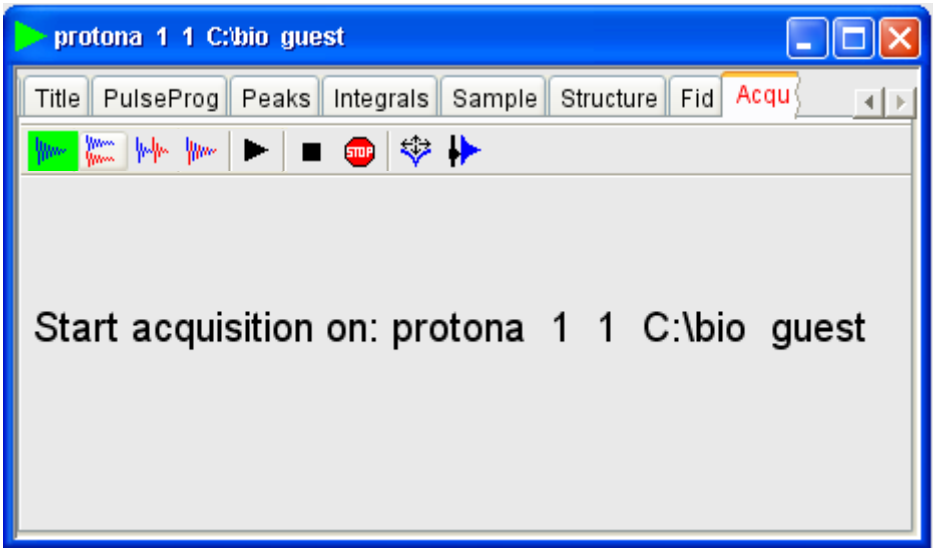


Figure 15.4

From here, you can start various acquisition commands like:

Start acquisition [***zg***]

■ Halt the acquisition [***halt***]

Stop the acquisition [***stop***].

Probe matching and tuning [***wobb***].

Interactive Parameter Adjustment [***gs***].

Data specific acquisition display allows you to open multiple acquisition display windows, one for each dataset.

Note that the ***Acqu*** tab is automatically activated when the acquisition is started from the TOPSPIN menu, toolbar or command line

15.4 Acquisition Status Bar

The acquisition can be followed and controlled from the acquisition status bar. Before you use the acquisition status bar, it must be configured from the User Preferences window. To do that:

1. Click ***Options*** → ***Preferences*** [***set***].
2. Click ***Acquisition status bar*** in the left part of the *User preferences* box. This will show the status bar items (see Fig. 15.5).

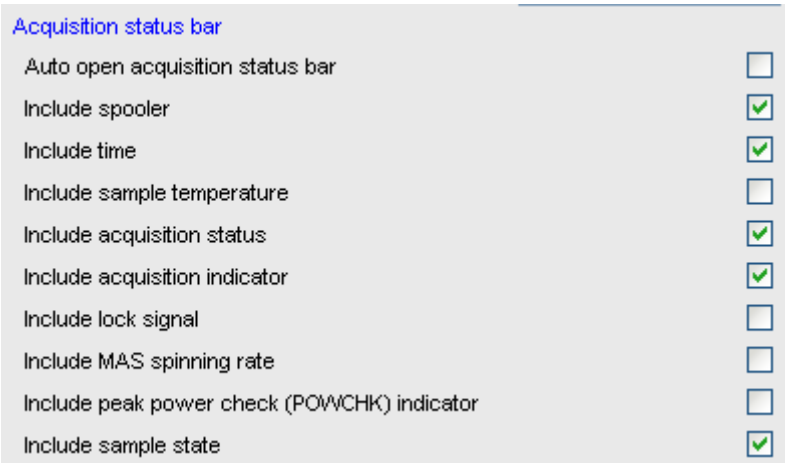


Figure 15.5

3. Check the desired entries.

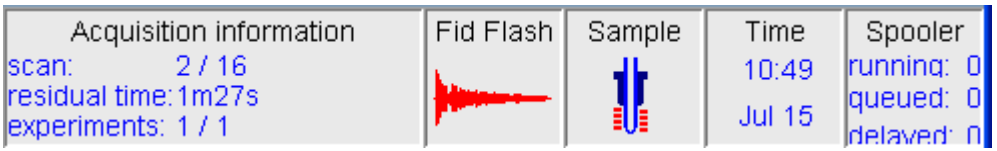
To switch the acquisition status bar on:

☞ Click ***Spectrometer → Acquisition Status Bar On/Off***

or

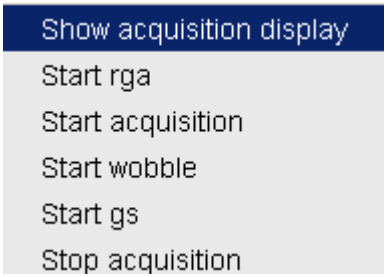
☞ Right-click in the status line at the bottom of the TOPSPIN window and choose the popup menu ***Acquisition Status Bar On/Off***

With the entries selected above, the right part of the status bar will look like this.



The acquisition status bar not only displays information, it also allows you to perform various actions, e.g.:

- Double-click the **Time** field to view detailed time and date information.
- Double-click the **Lock** field to open the lock display.
- Double-click the **Fid Flash** field to open the wobble display.
- Right-click the **Fid Flash** field to switch on/off FID flashing.
- Right-click the **Acquisition information** field to open the following popup menu:



from this menu, you can start various acquisition commands.

- Right-click the **VTU** field to open the following popup menu:



Clicking ***Options*** will open the following dialog box:

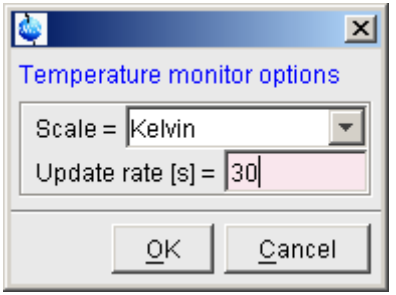


Figure 15.6

15.5 Command Queuing and Scheduling

TOPSPIN 2.0 and newer support command queuing (spooling) and scheduling. Acquisition commands like ***zg***, ***go***, ***rga*** and ***atma*** are automatically queued, if this feature is *on* (default *off*). This allows you, for example, to enter multiple ***zg*** commands on different datasets. Automatic queuing can be switched on as follows:

1. Click ***Options*** → ***Preferences***
2. In the User Preferences dialog:

   ☞ Enable *Auto-Spooling under Administration Items*

Processing commands can be queued with the command ***qu***. For example, the command sequence ***zg; qu xfb*** on a 2D dataset, will start an acquisition and, when this has finished, process the data.

Acquisition and processing commands can be scheduled with the command ***at***. Enter ***help qu*** or ***help at***, fo more details on the respective commands.

Queued commands can be viewed in the Spooling field of the acquisition status bar. Note that the spooling field must be activated in the User Preferences window (command ***set***).

15.6 Tuning and Matching the Probehead

Tuning and matching of conventional probeheads, (non ATM), is performed with the wobble procedure. To start this:

1. Enter ***wobb*** on the command line.

   The data window toolbar switches to the ***Acqu*** tab and the wobble window is opened (see Fig. 15.7).

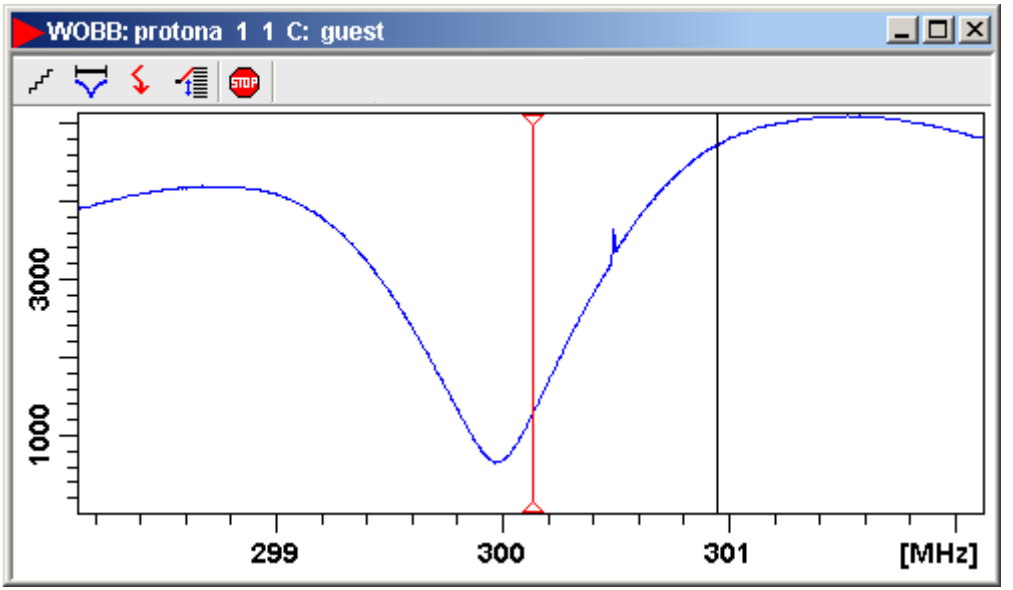


Figure 15.7

The buttons of the wobble toolbar have the following functions:

- Change the number of wobble steps [***wbst***].
- Change the wobble sweep width [***wbsw***].
- Change the wobble frequency.
- Switch to the next channel/nucleus (if available).
- Stop the wobble procedure.

2. Turn the tuning and matching knobs on the probehead until the wobble curve is exactly in the middle and its minimum reaches the zero line.

Automatic tuning and matching of ATM probeheads can be performed with the command ***atma***.

15.7 Locking

The lock display can be opened by clicking the button in the toolbar or entering ***lockdisp*** on the command line. The lock display window will appear (see Fig. 15.8).

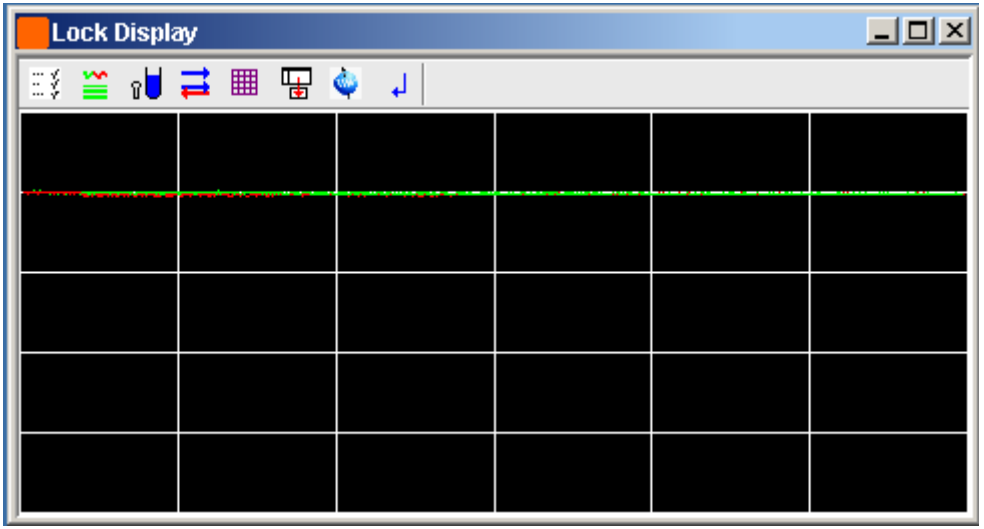


Figure 15.8

Here, you can view the lock signal, either during the lock-in procedure or, as shown above, after lock-in has been successful. At the top of the lock window the following buttons are available:

- Open the user preferences window [***set***].
- Toggle lock monitor mode.
- Lock the magnetic field [***lock***].
- Toggle lock display mode between *single* and *dual* color. Colors can be

set in the User preferences (command ***set***).

 Switch grid mode between *both*, *vertical*, *horizontal* and *off*.

 Make the lock display external.

 Put focus into TOPSPIN window.

 Close the lock display window.

Note that an external lock display window is independent from the TOPSPIN window. You can for example, minimizes TOPSPIN while keeping the lock display open.

The lock display can also be opened by double-clicking the lock field in the acquisition status bar (see par. 15.4)

The lock process can be started by entering ***lock*** on the command line. This command is described in the Acquisition Reference manual.

15.8 BSMS Control Panel

The BSMS control panel allows shimming, locking, sample handling and helium level measurement. To open this panel:

☞ Enter ***bsmsdisp*** on the command line

The BSMS Control Suite window will appear (see Fig. 15.9)

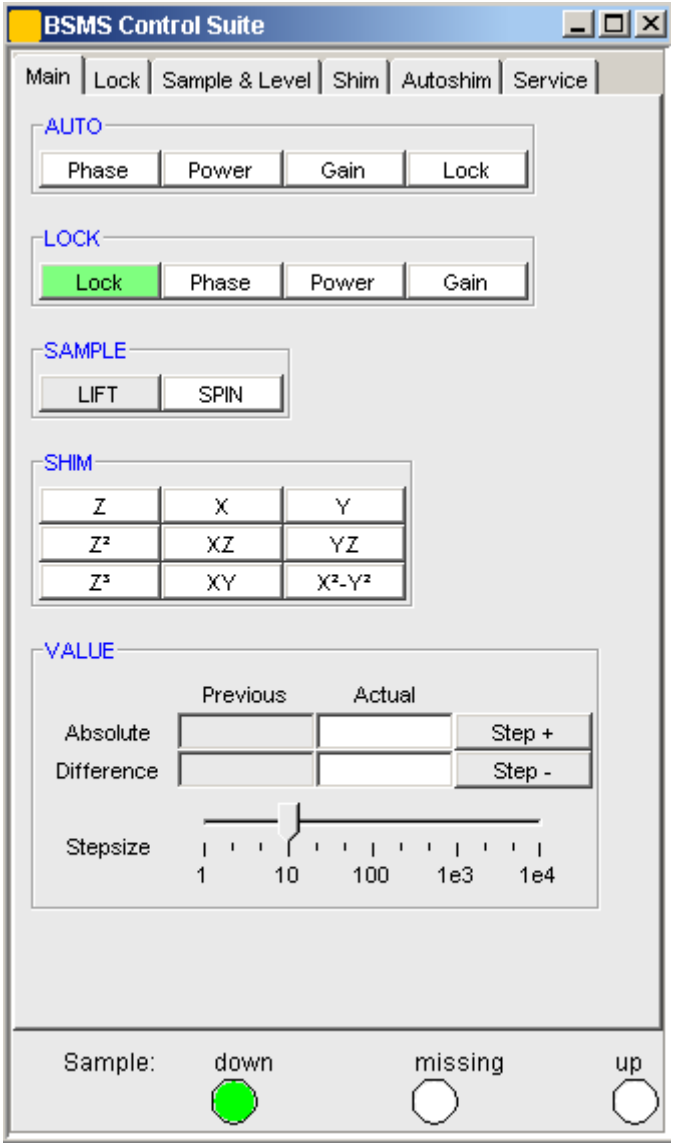


Figure 15.9

The individual functions BSMS control panel are described in detail in the Acquisition Reference manual.

15.9 Interactive Parameter Adjustment (GS)

Several parameters can be adjusted interactively, while observing the acquired FID. To start this:

☞ Enter ***gs*** on the command line.

A split window will appear showing:

- the FID display (see Fig. 15.10)
- the GS parameter adjustment dialog (see Fig. 15.11)

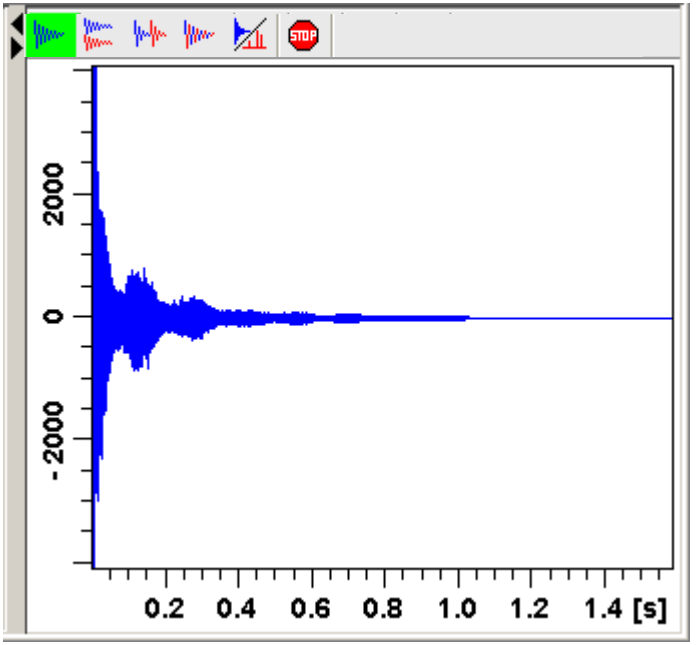


Figure 15.10

The buttons of the FID display are the same as for the acquisition command ***zg*** (see paragraph Fig. 15.10).

The GS parameter adjustment dialog offers tabs at the top of the window to select power, frequency, delay etc. The selected parameter is shown in the middle of the window. The slider at the right of the window allows you to change the selected parameter. The current value can be viewed and modified in the field below the slider. The sensitivity of the slider can be set in the field ***Sensitivity*** above the

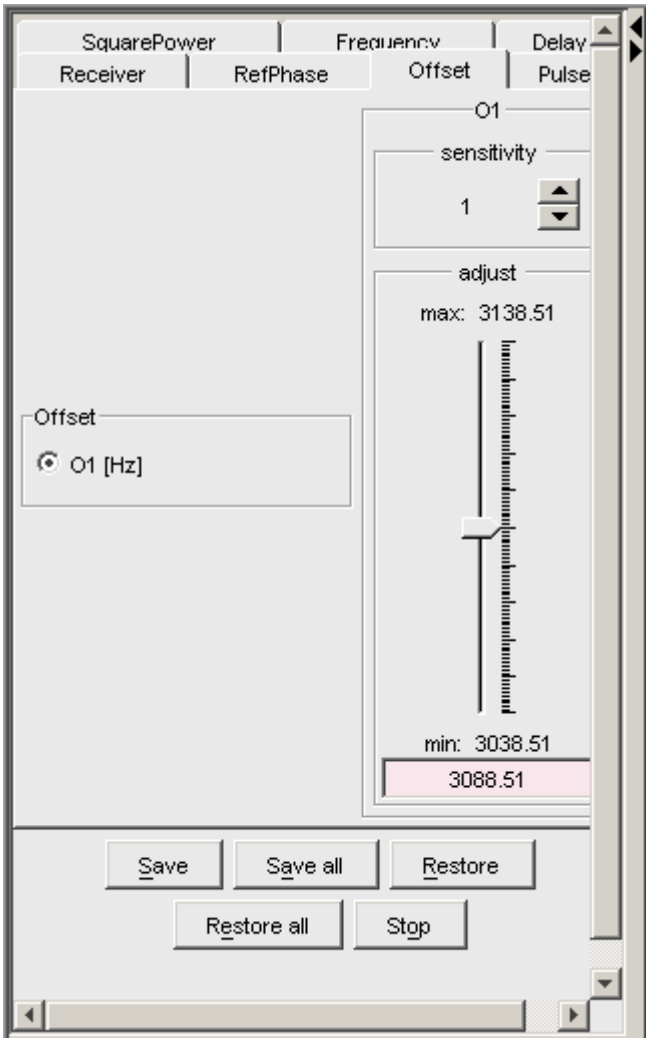


Figure 15.11

slider. The effect of the change can be viewed in the FID display, the right part of the window. This can be manipulated with the FID display buttons as described in chapter 15.10.

At the bottom of the window you find the following buttons:

- ***Save*** : Save the value of the current parameter.

- ***Save all*** : Save the values of all changed parameters.
- ***Restore*** : Restore the value of the current parameter.
- ***Restore all*** : Restore the value of all changed parameters.
- ***Stop*** : Stop the acquisition and quit the GS window.

15.10 Running an Acquisition

A typical acquisition is performed as follows:

1. Create a new dataset.
   a) Click ***File*** → ***New*** [***new***, ***Ctrl***+***n***].

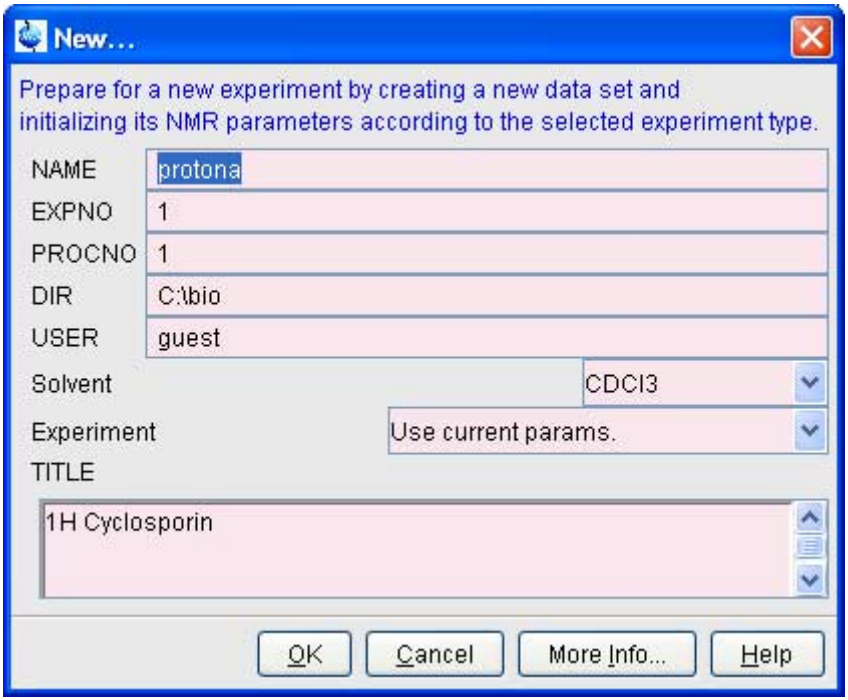


Figure 15.12

   b) Specify the datapath variables *name*, *expno*, *procno*, *dir* and *user*, select the desired ***Solvent*** and ***Experiment***, enter the ***Title*** and click ***OK***.

   The dataset will appear in the data field with no raw and no processed data

available.

2. Click the ***AcquPars*** tab to display the acquisition parameters.

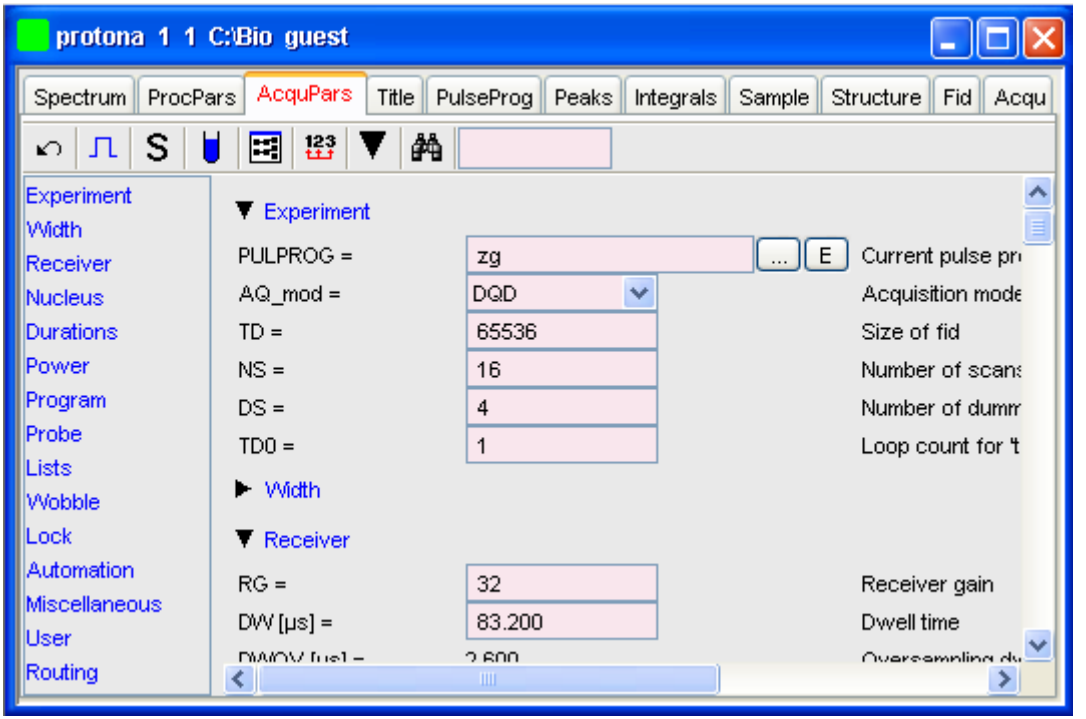


Figure 15.13

a) Optionally: click to show the pulse program parameters only.

b) Click the button to read the prosol parameters

or

Set the relevant parameters manually.

As an alternative to step 2, you can set the acquisition parameters interactively in the GS window (see par. 15.9).

3. To start the acquisition:

   - Click in the upper toolbar or enter ***zg*** on the command line.

The data window toolbar will automatically switch to the Acqu tab and the FID display window will appear:

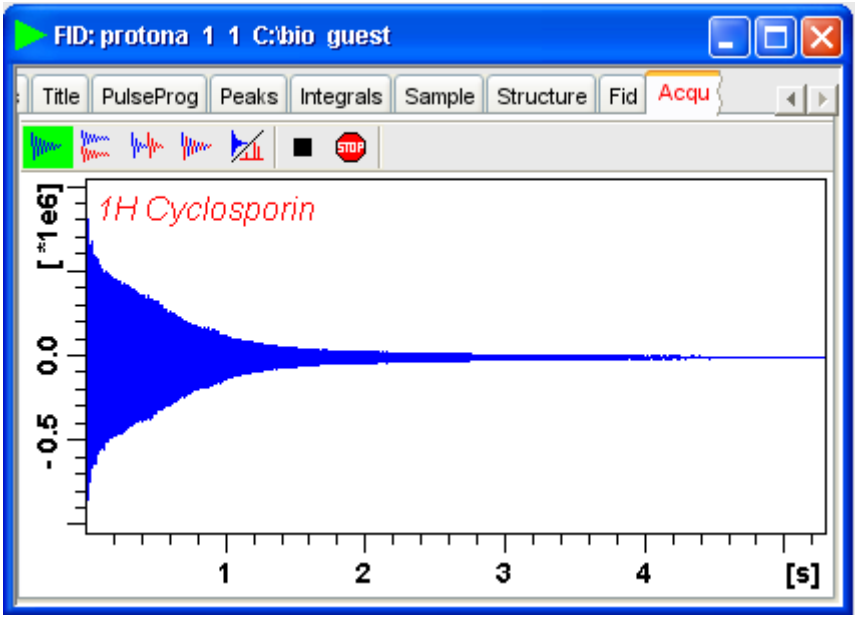


Figure 15.14

The buttons in the toolbar have the following functions:

Show FID in shuffled mode.

Show FID in unshuffled mode, horizontally arranged.

Show FID in unshuffled mode, vertically arranged.

Show FID in unshuffled mode, interleaved.

Switch between FID and spectrum.

Stop the acquisition [***stop***].

Halt the acquisition [***halt***].

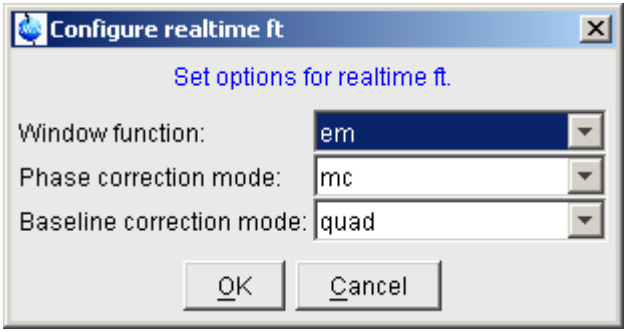
Clicking the button to switch to real time FT, turns the button green and opens two extra buttons:

 Switch between FID and spectrum.

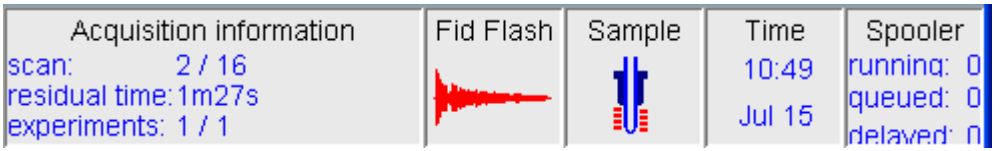
 Real time FT settings.

 Toggle calculation of peak with at 50%, 5.5% and 1.1% height (Shown as status parameters).

Clicking the  button opens the following dialog window:



The acquisition information will appear in the acquisition status bar at the bottom of the TOPSPIN window, for example:



4. When the acquisition has finished:

☞ Enter ***efp*** to process the FID.

The processed spectrum will be displayed in the data window that was opened upon creating the dataset (see Fig. 15.15).

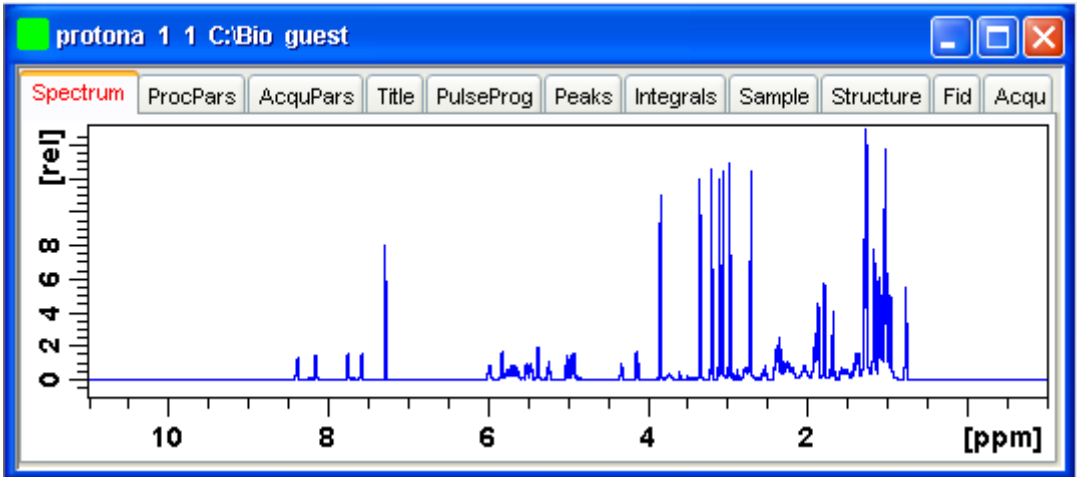


Figure 15.15

From here, the processed data can be analysed, printed and/or archived.

15.11 Shape tool

The Shape tool interface allows you to create/manipulate RF shapes and gradients.

To start the Shape Tool interface:

☞ Click ***Spectrometer → Shape Tool***

or enter **`stdisp`** on the command line.

The Shape Tool window will appear (see Fig. 15.16.). This consists of a toolbar, a command line and a split pane with a data section at the right and a parameter section at the left.

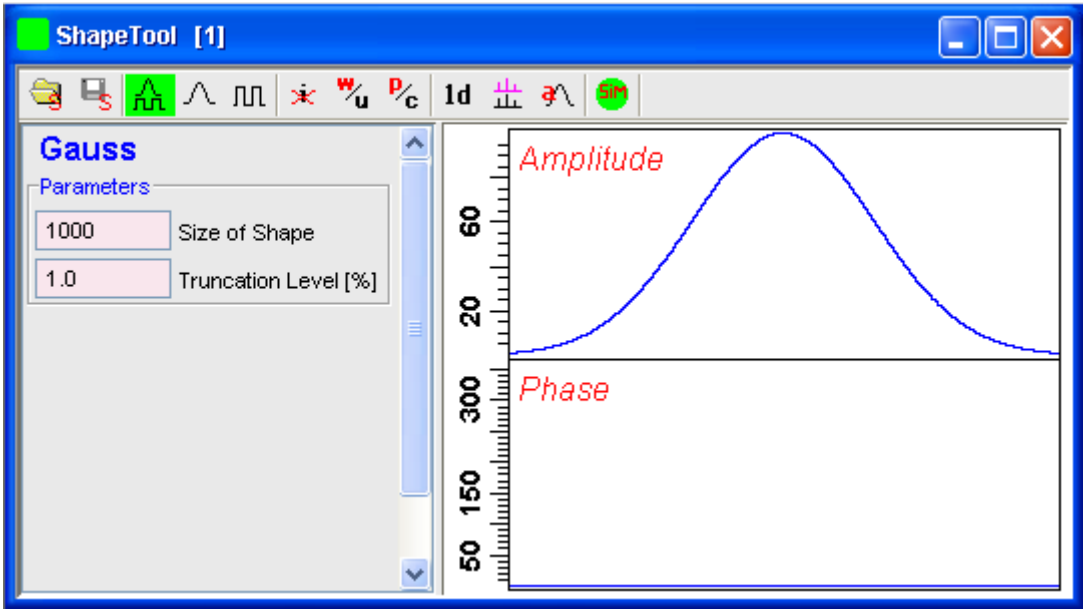
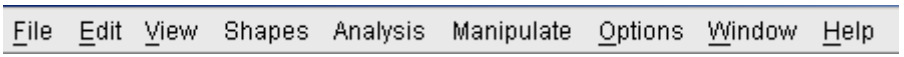


Figure 15.16

By default, a 1000 point Gauss shape is displayed with Truncation level 1.0.

The TOPSPIN menu is changed showing the additional ***Shapes*** and ***Manipulate*** menus and the adjusted ***File***, ***Analysis*** and ***Options*** menus.



Note that all functions of the interactive Shape Tool can also be performed non-interactively with the TOPSPIN command ***st***. This command must entered with the appropriate arguments on the command line while the associated dataset is displayed and selected.

A full description of the interactive and non-interactive Shapetool can be found under:

☞ Click ***Help*** → ***Manuals*** → [**Acquisition Application Manuals**] ***Shapetool***

Chapter 16

Configuration/Automation

16.1 NMR Superuser and NMR Administration password

During TOPSPIN installation, you are prompted to define:

- the username for the so called NMR Superuser. Under Windows this must be the name of an existing user. Under Linux it can also be a non-existing user, which is then automatically created by the installation program. After the installation, the NMR Superuser is the owner of all TOPSPIN program files. Logging in as this user allows you to remove these files, change file permissions etc. The name of the NMRSUPERUSER will be stored in the file:

  ```
  <tshome>/conf/nmrsuperuser
  ```

- the NMR Administration password to be used for TOPSPIN configuration commands. This password can be freely chosen and is not connected to any user. It is asked for by TOPSPIN commands like ***cf***, ***expinstall*** etc. The encrypted NMR Administration password is stored in the file:

  ```
  <tshome>/conf/nmradminpassword
  ```

Note that the NMR Superuser login password and the NMR Administration password have different purposes and are totally independent. Changing one of them does not affect the other.

How to Change the NMR Administration Password

The NMR Administration password can be changed as follows

Under Windows

1. Login as NMR Superuser or Administrator.
2. Open a Command Prompt.
3. Enter:

   <x>\perl\bin\perl <x>\prog\bin\installnmr <x> <NMRSUPERUSER>

   where <x> in the TOPSPIN installation directory.
4. Enter the old password and new password as requested.

Under Linux

1. Login as NMR Superuser or root.
2. Open a Shell.
3. Enter:

   <x>/prog/bin/installnmr <x> <NMRSUPERUSER>

   where <x> in the TOPSPIN installation directory.
4. Enter the old password and new password as requested.

If you don't know the old NMR Administration password, you can still define a new one. In that case, you have to delete the file:

```
<x>\conf\nmradminpassword
```

before you run the *installnmr* script.

16.2 Configuration

The main configuration steps are performed by the commands ***cf*** and ***expinstall***. They can be started from the:

- Command line
- ***Options*** → **Spectrometer tools** menu
- ***Spectrometer*** → ***Setup*** menu

However, the ***Spectrometer*** menu is only available after ***cf*** has been performed

once, choosing ***Installation for spectrometer***.

How to Perform a Default Configuration on a Datastation

A default configuration can be used on a datastation. It is automatically performed (no ***cf*** required) during the installation of TOPSPIN on a new computer, a new disk or in a new TOPSPIN installation directory. The default configuration name is *Bruker_default_av500* and corresponds to a Avance 500 MHz spectrometer.

For manual or interactive data processing, the automatic default configuration is sufficient. If, however, you want to use AU programs, you must execute ***expinstall*** once, selecting *Installation for Datastation (Default).*

How to Perform a Customized Configuration on a Datastation

If you want to configure your datastation according to a spectrometer other than default, you must first copy the configuration directory:

<tshome>/conf/instr/<instrum>

from that spectrometer to the datastation. Here:

<tshome> is TOPSPIN home, the directory where TOPSPIN is installed. Note that this can be different on the spectrometer than on the datastation.

<instrum> is the configuration name.

After copying the configuration directory, you have to perform ***expinstall*** as follows:

- Click ***Spectrometer*** → ***Setup*** → ***Experiment installation*** or enter ***expinstall*** on the command line

Follow the instructions on the screen. In successive dialog boxes check/select the options below and click ***Next*** to continue:

- *Installation for Datastation (Customize)*
- *High Resolution Systems*
- The configuration name as it was copied from your spectrometer
- The items you want to install
- Select the desired printer and paper format for the parameter sets
- The spectrometer frequency, acquisition mode and pre-scan-delay

In the last dialog box, click ***Finish***. The installation of the selected items, will start

now. Wait until this process has finished.

For more details on ***expinstall***, please refer to the description of this command in the Acquisition Reference manual.

16.3 Parameter set conversion

The command ***paracon*** changes the basic frequency in parameter sets. This allows you to use parameter sets which were created on a spectrometer with a different frequency. It opens dialog box shown in Fig. 16.1

Here you can setup a list of available parameter sets. You can select Bruker and/or User defined parameter sets and use a match string. The matching parameter sets appear in the right part of the dialog box. To start the conversion, select one or more parameter sets and click ***OK***.

16.4 Automation

How to Install AU Programs

To install AU programs, you have to run the command ***expinstall*** (see chapter 16.2).

How to Open the AU Program Dialog Box

To get a list of all AU programs, enter ***edau*** or:

1. Click ***File*** → ***Run...***
2. Click ***Execute an AU program*** in the appearing dialog box.
3. Click ***OK***

A dialog box showing either the Bruker defined or User defined AU programs. Fig. 16.2 shows a dialog box with two User defined AU programs.

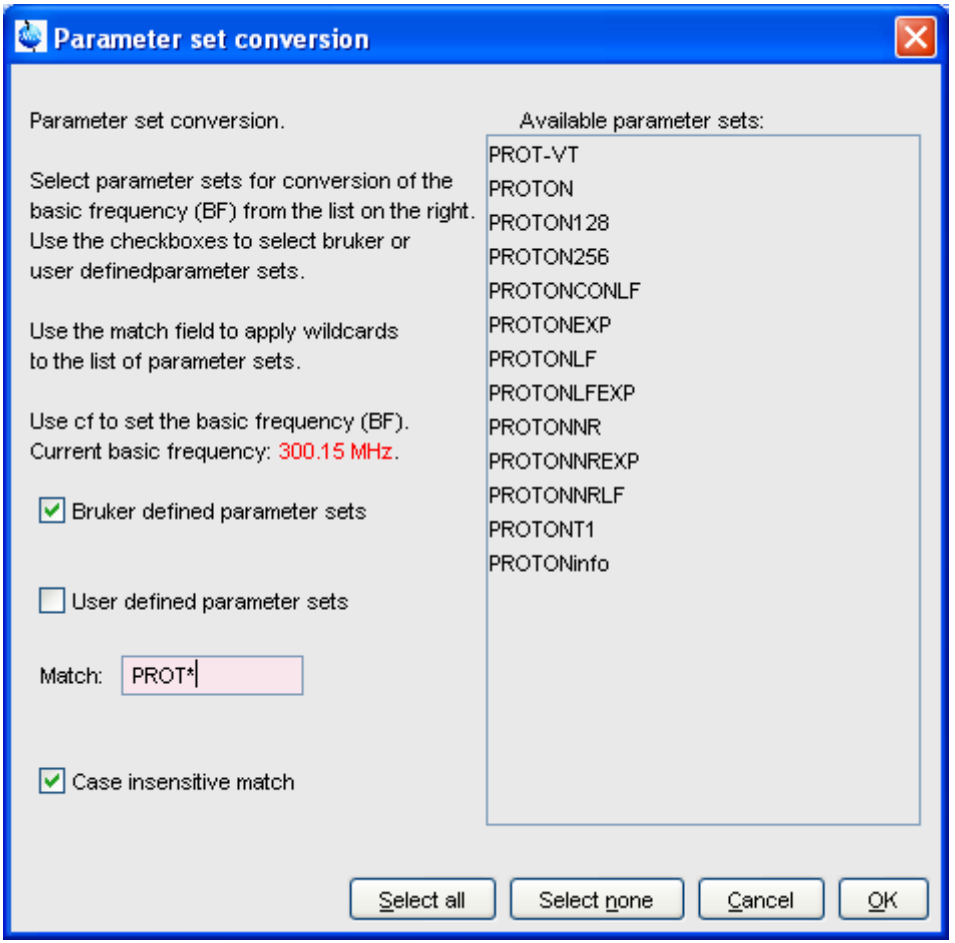

Parameter set conversion
Parameter set conversion.
Select parameter sets for conversion of the basic frequency (BF) from the list on the right. Use the checkboxes to select bruker or user definedparameter sets.
Use the match field to apply wildcards to the list of parameter sets.
Use cf to set the basic frequency (BF).
Current basic frequency: 300.15 MHz.
Bruker defined parameter sets
User defined parameter sets
Match: PROT*
Case insensitive match
Available parameter sets:
PROT-VT
PROTON
PROTON128
PROTON256
PROTONCONLF
PROTONEXP
PROTONLF
PROTONLFEXP
PROTONNR
PROTONNREXP
PROTONNRLF
PROTONT1
PROTONinfo
Select all
Select none
Cancel
OK

Figure 16.1

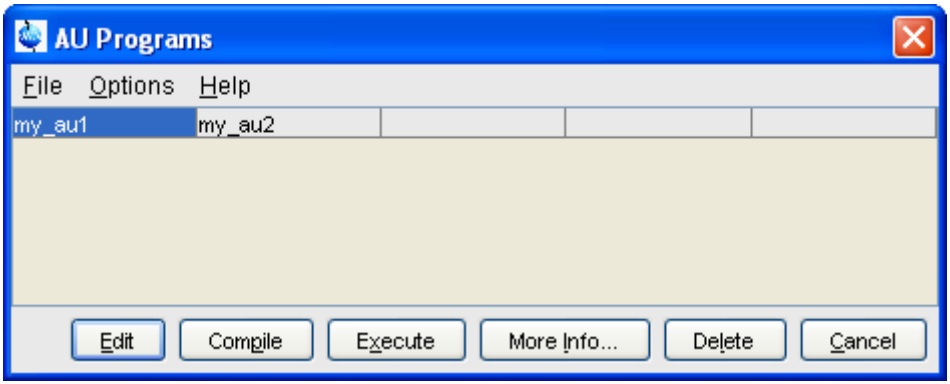


Figure 16.2 List with two User defined AU programs

Note that Bruker AU programs are only shown if the command ***expinstall*** has been executed once, after the installation of TOPSPIN.

How to Switch to the List of User defined AU Programs

☞ Click ***Options*** → ***User defined*** in the AU program dialog box

How to Switch to the List of Bruker defined AU Programs

☞ Click ***Options*** → ***Bruker defined*** in the AU program dialog box

How to Define the AU Programs Source Directory

1. Click ***Options*** → ***Manage Source Directories*** in the AU program dialog box
2. In the field **AU Programs**: Add or modify AU program source directories

How to Create an AU Program

1. Click ***File*** → ***New*** in the AU program dialog box.
2. Enter the AU program lines in the edit field of the appearing dialog box.
3. Click ***Save as...***to store the AU program under a new name.
4. You will be prompted to compile the AU program: click ***OK***.

Alternatively, you can enter ***edau <name>*** on the command line to create the AU program <name>.

How to Edit an Existing AU Program

1. Double-click the AU program name in the AU program dialog box

   or

   Click the ***Edit*** button to edit the highlighted AU program.
2. Modify the AU program according to you wishes.
3. Click ***Save*** to store the AU program under the name shown in the title bar.
4. You will be prompted to compile the AU program: click ***OK***.

Alternatively, you can enter ***`edau <name>`*** on the command line to edit the AU program <name>.

How to Execute an AU Program

1. Select the AU program in the AU program dialog box.
2. Click the ***Execute*** button.

Alternatively, you can enter ***`<name>`*** or ***`xau <name>`*** on the command line to execute the AU program <name>.

If the AU program has not been compiled, compilation is automatically performed before the execution starts.

How to Delete an AU Program

1. Select the AU program in the AU program dialog box.
2. Click ***File*** → ***Delete*** or click the ***Delete*** button.

How to Show Comments (short descriptions) in the AU Program List

To switch on/off the comments in the AU program list:

☞ Click ***Options*** → ***Comment on/off*** in the AU program dialog box.

A comment is a short description of the AU program which is also part of the AU program header.

Chapter 17

Regulatory Compliance

TopSpin complies with the FDA 21 CFR Part 11 regulations. Please read the , accessible under ***Help*** → ***Manuals*** → [**Good Laboratory Practice**] ***21 CFR Part 11 compliance***. This chapter describes the respective functionalities provided by TOPSPIN in detail.

17.1 Audit Trails

A TOPSPIN data set consists of acquisition (= raw) data and processed data. These are stored in a directory tree with the following structure:

<*dir*>\data\<*user*>\nmr\<*name*>\<*expno*>\pdata\<*procno*>

The acquisition data are stored in the *expno* sub-directory and the processed data are stored in the *procno* subdirectory.

17.1.1 The raw data audit trail

Each *expno* sub-directory contains a text file *audita.txt*, the audit trail of the raw data. This reflects the acquisition state of the raw data, and contains a checksum for the file itself (*audita.txt)* and one for the raw data file (*fid* or *ser*). The latter links the audit file with the raw data. By means of the checksums, any illegal manipulation of the audit file or the raw data file can be detected, using the TOPSPIN commands **`audit`** or **`auditcheck`**. Whenever an acquisition is started, the

possibly existing audit file is overwritten by a new one, belonging to the new raw data file. By default, the user is warned when the current dataset already contains raw data, thus preventing accidental overwriting (The option “Override existing fid without inquiry” is, by default, off (see ***Options*** → ***Preferences*** → ***Acquisition***).

17.1.2 The processed data audit trail

Each *procno* sub-directory contains a text file `auditp.txt`, the audit trail of the processed data. It reflects the processing state of the processed data and contains a checksum for the file itself (`auditp.txt`), and a checksum for the real processed data files (`1r`, `2rr`, `3rrr`, ...). The latter links the audit file with the processed data. By means of the checksums, any illegal manipulation of the audit file or the processed data file can be detected, using the TOPSPIN commands ***`audit`*** or ***`auditcheck`***. Whenever a processing command is performed, the current audit file is updated with this command and its associated parameters. When processing starts from scratch (from a raw data file), the existing audit file is overwritten. As such, the processed data can always be regenerated from raw data by applying the commands and parameters listed in the audit trail.

If the laboratory management does not allow data files or audit trails to be deleted, a respective saving procedure must be established. For this purpose, TOPSPIN provides data copying commands, which may be called in a user defined macro or AU program, before a new acquisition or processing starts.

17.1.3 Viewing audit trails

Since audit trails are regular ASCII text files, they can be viewed or printed with any text editor, outside of TOPSPIN. Within TOPSPIN, you can use the command ***`audit`*** for this purpose. This opens the dialog box show in Fig. 17.1.

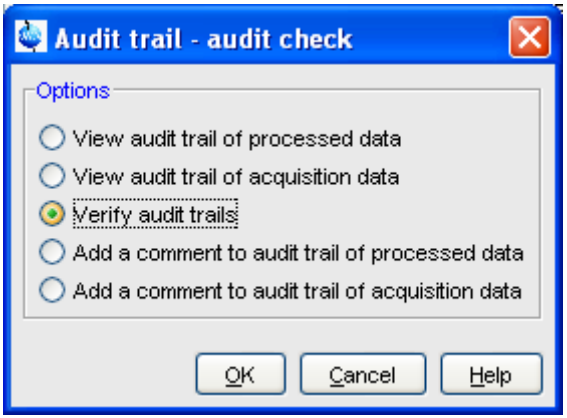

Audit trail - audit check
Options
View audit trail of processed data
View audit trail of acquisition data
Verify audit trails
Add a comment to audit trail of processed data
Add a comment to audit trail of acquisition data
OK
Cancel
Help

Figure 17.1

The first two entries allow you to view the audit trail files. The third entry performs an audit trail check, i.e. a data consistency check. If both raw and processed data are consistent, you will get the message shown in Fig. 17.2.

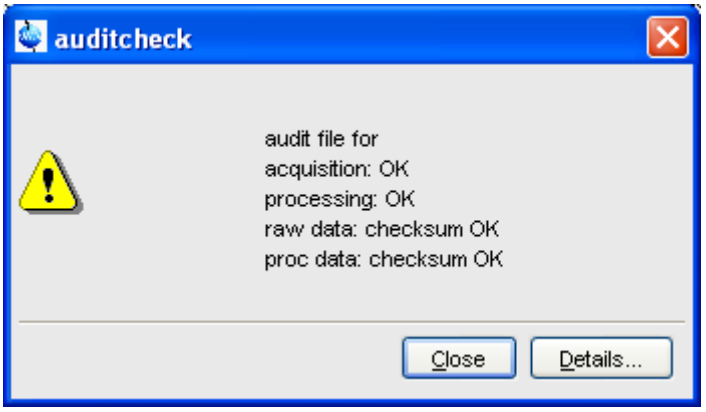


Figure 17.2

If the data have been manipulated outside of TOPSPIN, e.g. with third party software, the checksum will be inconsistent. Fig. 17.3 shows the message for incon-

sistent processed data.

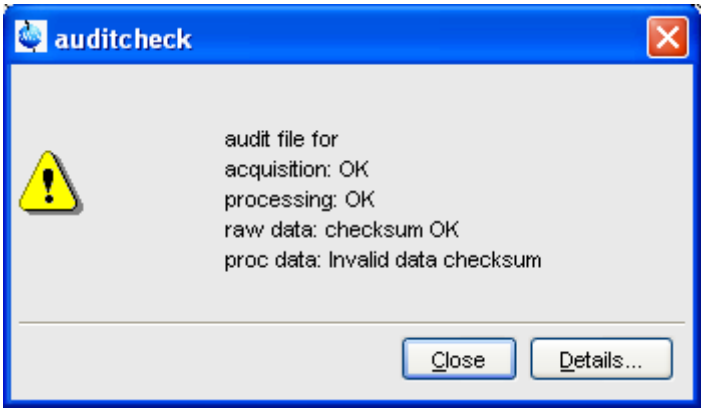


Figure 17.3

The fourth and fifth entry in Fig. 17.1 allow you to add a comment to the raw or processed audit trail files, respectively.

17.1.4 Audit trail contents

The contents of an audit file is grouped in the following way:

(NUMBER, WHEN, WHO, WHERE, PROCESS, VERSION, WHAT)

These entries have the following meaning:

NUMBER

Running number of an entry, starting with 1.

WHEN

Date of the entry, e.g. <2004-03-30 10:55:36.171 +0200>, where the last value represents the offset in hours to Universal Time (UTC).

WHO

The user logged in, at the time the entry was generated. It has one of the two forms: <user1> or <user1/user2>. <user1> is always the user who is logged into the operating system (Windows or Linux user), and who started TOPSPIN. <user2> only appears, if the NMR administrator has setup an internal TOPSPIN user administration, and the option *Enforce "login" for working with*

TOPSPIN in the User Administration dialog is enabled (see below, command ***uadmin***). In this case <user2> is the current internal TOPSPIN user.

WHERE

The network name of the current computer, e.g. <EOS2>.

PROCESS

The TOPSPIN process (module) which performed the acquisition or processing.

WHAT

The type of acquisition or data manipulation performed.

Note that if only the entries NUMBER, WHEN, WHO, WHERE, WHAT be present, then the audit trail was created by TOPSPIN 1.3 or older.

17.1.5 Adding a comment to an audit trail

Audit trail entries are normally generated automatically by a respective acquisition or processing command. However, a user can also add a comment manually, using the ***audit*** command. This will generate a regular entry, the comment will appear under the WHAT section and is preceded by the tag "*user comment*:".

You may also add a comment to the raw data or processed data audit trail from an AU program, using the macros AUDITCOMMENTA(comment) or AUDITCOMMENTP(comment), respectively. Alternatively, you can store the comment in a file `auditc.txt` in the *expno* or *procno* directory, and use the macros GDCHECK_RAW or GDCHECK

17.1.6 Auditing user-defined data manipulations

When manipulating a data file with a user-defined algorithm, e.g. by means of an AU program or external program, the data file and the respective audit trail become inconsistent (detectable with the command ***auditcheck***), and the data set is no longer compatible with regulations. In order to solve this problem, TOPSPIN provides a function *CheckSumFile*, which adds the correct data checksum to the audit trails, and a function *AuditAppend* for additional text (an alternative to the comment function described above). These functions are described in the AU manual which can be opened by clicking ***Help*** → ***Manuals*** → [**Programming Manuals**] ***AU programming.***

17.1.7 Audit Trails in JCAMP-DX and ZIP archives

The TOPSPIN commands ***tojdx*** and ***tozip*** allow you to store a data set into a single file in the internationally standardized ASCII-type JCAMP-DX format or in the well-known ZIP format, respectively. Both storage formats retain the audit trails. When unpacking such files with ***fromjdx*** or ***fromzip***, respectively, the original data set in standard Bruker format is restored. The command ***auditcheck*** may be used to check whether the data are still consistent. If, for example, JCAMP-DX or ZIP file have been manipulated, the data might not be consistent.

17.2 Electronic Signatures

17.2.1 Signing a data set

The command ***esign*** adds an electronic signature to the raw data or to the processed data of a data set. It opens a dialog where you can select the data component to be signed, the signature meaning and, optionally, add a comment. ***esign*** requires that the NMR administrator has set up a list of users who are allowed to sign a data set, along with definitions of signature *meanings* (e.g. review, approval). See below for details, command ***uadmin***.

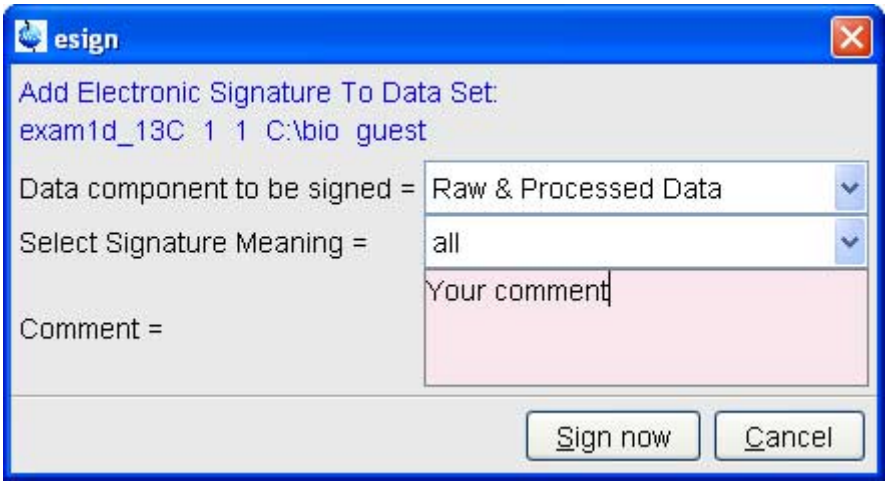


Figure 17.4

17.2.2 Structure of a signature

In TOPSPIN, an electronic signature is realized as a special entry appended to the audit trail of the raw or processed data. It is therefore linked with the data and protected against manipulations just like any other audit trail entry. Signatures can be viewed with the command ***audit***. An electronic signature consists of the following items:

USER ID

The ID of the user logged in at the time ***esign*** was executed. This is either the user who was logged into the operating system (Windows or Linux user), and who started TOPSPIN, or the TOPSPIN internal user. Which of these two modes is applied depends on how the NMR administrator configured TOPSPIN: If the option *Enforce "login" for working with* TOPSPIN is disabled (see below, command ***uadmin***), the first mode is active, otherwise the second.

What is the difference between the modes?

- In the first case, the System User (= Windows or Linux user) who started TOPSPIN signs the data set. Prior to signing, ***esign*** requests this user's password, which is administrated by the operating system (OS). No internal TOPSPIN user management plays a role. *Advantage:* This mode is entirely OS compliant. *Disadvantages:* a) TOPSPIN termination/restart is required when a different user wants to sign data (alternatively several licenses would admit simultaneous TOPSPIN sessions). b) All TOPSPIN users must have an OS login.
- In the second case, any TOPSPIN internal user who is enabled by the NMR administrator (with ***uadmin***) may sign. *Advantage:* Convenient and easy usage. *Disadvantage:* TOPSPIN internal user management is required (internal users and their passwords).

USER NAME

The complete name of the signer as specified by the NMR administrator during user administration (command ***uadmin***).

SIGNATURE MEANING

The meaning of a signature, e.g. *Review* or *Approval*. A user may only select meanings that were assigned to him by the NMR administrator during user administration.

SIGNATURE COMMENT

Any text.

17.2.3 Displaying the electronic signature in the data window

The electronic signature can be displayed in the data window by setting the corresponding display component. To do that:

1. Right-click in the data window and choose ***Display Properties...*** [***.dopt***].
2. Check ***Electronic Signature*** in the appearing dialog box and click ***OK***.

The electronic signature will appear, at the upper left corner, below the title.

17.2.4 Plotting the electronic signature

When plotting a dataset using TOPSPIN's plot editor (commands ***plot*** and ***autoplot***), an electronic signature is automatically plotted (unless this feature is disabled), if the last entry of the audit trail of the data to be plotted is an electronic signature. This ensures that after signing no more data manipulations have been performed.

17.2.5 Multiple signatures

The command ***esign*** may be applied several times to a data set, for instance if two persons (say an operator and an administrator) must sign in accordance with company regulations.

17.2.6 Validity and security of signatures

TOPSPIN electronic signatures of data sets must not be confused with digital signatures as defined in applicable law. Digital signature laws are usually country dependent. They require the administration of passwords (more general: electronic keys which authenticate the owner of the document) to be performed by authorized trust centers. In contrast, TOPSPIN uses OS-encrypted passwords or internal user passwords encrypted by TOPSPIN itself.

For this reason, a Standard Operating Procedure (SOP) of the company or institution that wishes to apply TOPSPIN signatures must exist defining the role of TOPSPIN signatures.

For this reason, companies and institutions that want to apply TOPSPIN signatures

must have a Standard Operating Procedure (SOP), which defines the role of these signatures.

Note that digital signatures complying with respective laws requires special software, and the involvement of trust centers. Bruker refers to the respective commercial software for this purpose.

17.3 Password Controlled Login Identification

17.3.1 Definition of an internal user

In TOPSPIN, the NMR administrator may set up a list of *internal* TOPSPIN *users*. An internal user need not have a user account for the operating system and is only known to TOPSPIN. Such a user is characterized by the following items:

USER ID

A short unique string of characters identifying a user (e.g. guest)

USER NAME

A long string of characters, usually the full name of a user (e.g. Franz J. Maier)

SIGNATURE MEANINGS

A list of items separated by comma (e.g. Approval, Review), an empty string or the special string "-NONE-". In the latter two cases, this user cannot electronically sign data. In all other cases, the user is allowed to sign. The ***esign*** dialog allows the user to select one of the items to specify the meaning of the signature.

PASSWORD

A password for this user, required for using TOPSPIN and for applying an electronic signature.

17.3.2 How to set up internal users

In order to define or modify the list of internal users:

☞ enter the command ***uadmin***

or

☞ Click ***Options → Preferences → Administration items***

Click the ***Change*** button to the right of the object *Setup users for TopSpin-internal login/logoff and esign.*

You will be prompted for the NMR administrator password. A dialog will appear.

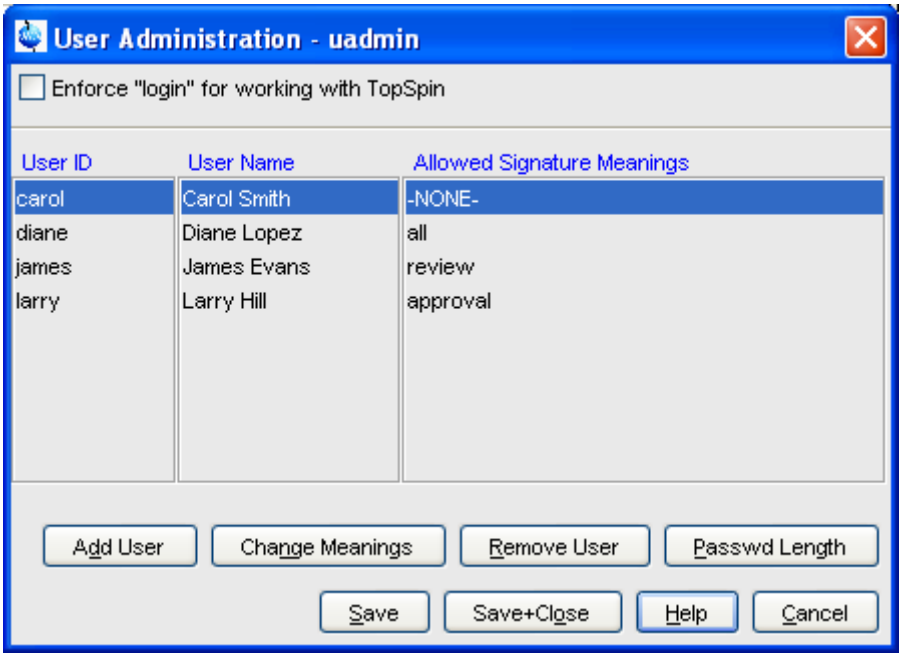


Figure 17.5

where you can add, remove and/or modify users

17.3.3 How to change the internal user password

To change the password of the internal user:

☞ enter ***chpwd*** on the command line

or

☞ Click ***Options → Administration → Change internal user password***

and enter the new password twice, as requested.

17.3.4 Login/Logoff

The ***uadmin*** command allows the administrator to make a TOPSPIN internal user mandatory. To do that, enable *Enforce "login" for working with TopSpin* at the top of the dialog, click ***Save+Close*** and restart TOPSPIN. After the restart, a login prompt will be displayed and TOPSPIN cannot be used without entering an internal user and his password.

To log off the internal user:

☞ enter ***logoff*** on the command line

or

☞ Click ***Options → Administration → Log off***

and enter the user name and password as requested.

If TOPSPIN internal user is not mandatory, i.e. the entry *Enforce "login" for working with TopSpin* is disabled, you are not prompted to login after TOPSPIN startup. You can, however, still login as internal user with the command ***login***.

17.3.5 Locking TOPSPIN's Graphical User Interface

TOPSPIN can be blocked, such that it does no longer accept user input via mouse or keyboard. To do that:

☞ enter ***lockgui*** on the command line

or

☞ Click ***Options → Administration → Lock TopSpin user interface***

A window will appear (see Fig. 17.6) indicating the locked status and offering but-

tons to unlock.

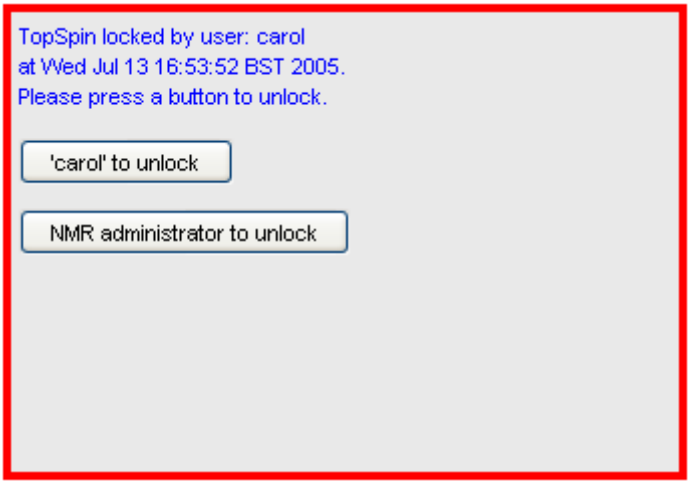

TopSpin locked by user: carol
at Wed Jul 13 16:53:52 BST 2005.
Please press a button to unlock.
'carol' to unlock
NMR administrator to unlock

Figure 17.6

Only the current user or the NMR Administrator can unlock the user interface. While TOPSPIN is locked, all background activity such as data acquisition and processing continue.

For safety reasons TOPSPIN can be forced to execute ***`lockgui`*** automatically when no commands from the command line, menus or tool buttons have been entered for a certain period of time (for instance because the current user has left). In order to enable automatic locking

1. Click ***Options*** → ***Preferences*** [***`set`***]
2. Click ***Administration Items*** in the left part of the dialog box.
3. Click the ***Change*** button to the right of the object *Automatic locking of TopSpin when idle time exceeded*.
4. Enter the maximum allowed idle time (in minutes) in the dialog and click ***OK***.

Chapter 18

Remote Control

18.1 Remote control

TOPSPIN supports remote control. This means, for example, that you can control your spectrometer from any PC in the laboratory network or, over the internet, from your PC at home. Using your local TOPSPIN interface, you have access to the remote data directories and remotely running TOPSPIN commands. Furthermore, in TOPSPIN 1.3 and newer, ICON-NMR is web-enabled which means it can be controlled from any web browser which is networked to the spectrometer. Note that remote access is operating system independent.

18.2 How to Establish a Remote Connection from your PC

In order to establish a remote connection, you have to perform a few steps, both on the local and on the remote system. Note that the local system is the computer you are sitting at, and the remote system is the computer you are connecting to. Up to 5 local systems can connect to TOPSPIN on a remote system.

18.2.1 Setup the remote system

The remote system must be enabled for remote access and, furthermore, individual data directories must be exported.

Enable the system for network access

1. Log in on the remote system
2. Start TOPSPIN
3. Click ***Options*** → ***Preferences*** [`set`]
4. Click ***Miscellaneous*** in the left part of the dialog box.
5. Click the ***Change*** button to the right of the object *Configure remote access.*
6. Enter the Administration password as requested
7. In the appearing dialog box (see Fig. 18.1):
   a) Click ***Remote Access Enable***
   b) Click ***Add*** and enter the data directories that you want to export for remote access, e.g.: `C:\bio` and click ***OK.***
   c) Click ***OK*** to close the dialog.

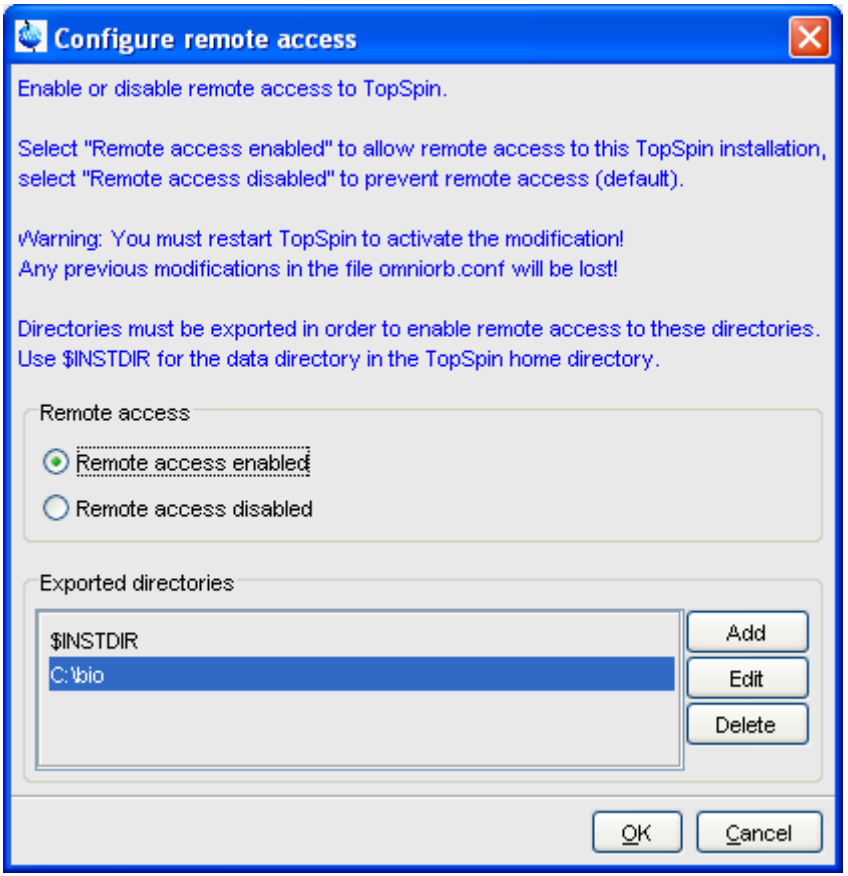

Configure remote access
Enable or disable remote access to TopSpin.
Select "Remote access enabled" to allow remote access to this TopSpin installation, select "Remote access disabled" to prevent remote access (default).
Warning: You must restart TopSpin to activate the modification!
Any previous modifications in the file omniorb.conf will be lost!
Directories must be exported in order to enable remote access to these directories. Use $INSTDIR for the data directory in the TopSpin home directory.
Remote access
Remote access enabled
Remote access disabled
Exported directories
$INSTDIR
C:\bio
Add
Edit
Delete
OK
Cancel

Figure 18.1

8. Click ***OK*** to save and close the preferences dialog.
9. Restart TOPSPIN.

A list of exported directories is stored the file:

```
<tshome>/prog/server/export.conf
```

Now a running TOPSPIN on this system can be accessed from any computer in the network.

Identify the port number

To identify the TCP/IP port number used by TOPSPIN:

1. Start TOPSPIN
2. Enter ***hist***
3. Look for the line

   To connect to this TOPSPIN .... use host=<xxxx>., port=<yyyy>

   in the upper part of the dialog window. The number at the end of this line (<yyyy) is the desired port number, which must be used to set up the local system (see chapter 18.2.2). By default, this is port number 5500. Only if this port is already used by a program other than TOPSPIN, a different port is used.

Export data directories

1. Log in on the remote system as Administrator (windows) or root (Linux).
2. Edit the file `<tshome>/prog/server/export.conf`

   By default, this file contains the lines:

   ```
   EXPORTMODE=ALL
   $XWINNMRHOME
   ```

   This first entry should be left as it is. The second entry exports the data directory <tshome>/data for remote access. By default, that this is the directory that contains the Bruker example datasets.
3. Add the data directories that you want to export for remote access, e.g.:

   ```
   C:\bio
   D:\nmr
   ```

   for the directories `C:\bio\data` and `D:\nmr\data`, respectively. Please use a separate line for each entry!
4. Save the file `export.conf` and close the editor.

18.2.2 Setup the local system

Define the remote system

1. Log in on the local system
2. Start TOPSPIN
3. Click ***Options*** → ***Preferences*** [***set***].
4. Click ***Miscellaneous*** in the left part of the dialog box.

5. Click the ***Change*** button at the entry *Setup remote systems*. In the appearing dialog (see Fig. 18.2),

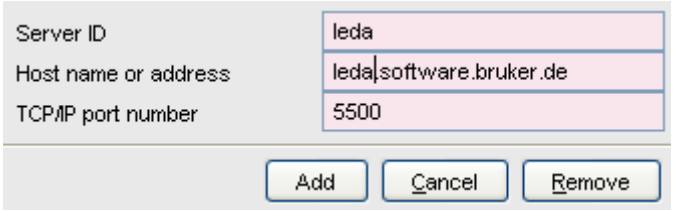


Figure 18.2

enter the following information:

- Server ID: an arbitrary name for the remote system
- Hostname or address: the hostname or IP address of the remote host
- TCP/IP port number of the remote TOPSPIN as identified in chapter 18.2.1.

6. Click ***Add*** to add the remote host.
7. Click ***OK*** to save the changes and close the dialog.

Note that you can define multiple remote systems, for example different spectrometers in your laboratory.

Connect to the remote system

1. Click ***Options*** → ***Remote connection...***
2. Select the desired *Remote system* from the appearing dialog box and click ***OK***.

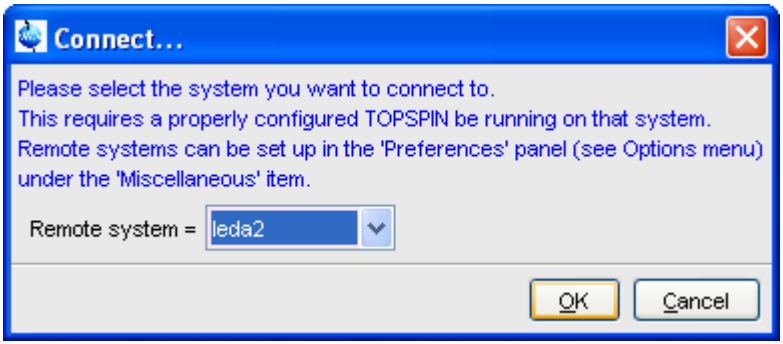

Connect...
Please select the system you want to connect to.
This requires a properly configured TOPSPIN be running on that system.
Remote systems can be set up in the 'Preferences' panel (see Options menu)
under the 'Miscellaneous' item.
Remote system =
leda2
OK
Cancel

Figure 18.3

Now you are prompted for a user and password (**both case sensitive**) on the remote computer.



Figure 18.4

The TOPSPIN browser will show the exported data directory trees of the remote system. You are now ready to acquire, process or analyse remote data.

18.2.3 Setup the firewall

A remote system in a network can be protected by a firewall. Any firewall between the local and remote TOPSPIN must be configured for TOPSPIN remote access.

If the remote PC is running under Windows XP with Service Pack 2, the Windows Firewall is, by default, installed and running. Consider the following possibilities:

Firewall on PC with Windows XP-SP2, Topspin installed

If TOPSPIN is installed, the firewall is probably configured for TOPSPIN remote access [1]. If it is not or you are not sure, you can configure it as follows:

1. Click **Start → Programs → Bruker TOPSPIN → TOPSPIN 2.0 → Bruker Utilities**
2. Click **Miscellaneous**
3. Double click **Command Prompt**
4. In the Command Prompt window, enter:

```
cd prog\bin\utilities\Miscellaneous
setfirewall.cmd auto
```

Firewall on PC with Windows XP-SP2, no Topspin installed

Configure the firewall as described in the Installation Guide for Windows XP.

On all other systems, the firewall must be configured manually by the network administrator. To do that view the file:

```
<tshome>/prog/server/corba.conf
```

and open the ports specified here, incremented by 50.

For more information, please refer to the installation guides for Windows or Linux or inspect the contents of the file `corba.conf`.

Note that the firewall must be configured for TOPSPIN:

- spectrometer control
- remote access

TOPSPIN can be used for processing/analysis on a local datastation, even if it is not registered on the firewall. However, you will get a few Security Alert messages during startup.

1. During TOPSPIN installation, you can choose to automatically configure the firewall or not. PC's delivered by Bruker Germany, always have the firewall configured for TOPSPIN.

18.3 How to Make a Remote Connection without a Local License

TOPSPIN requires a license to operate on your local computer. However, you can make a remote connection without a local license.

To do this, you have to start TOPSPIN as follows:

1. Open a Windows Command Prompt or Linux Shell.
2. Go to the TOPSPIN installation directory.
3. Enter ***topspin -client***
4. TOPSPIN will start up and show an empty data field but no browser. Before startup you will get the error message: "*The program failed to communicate with local ....*". Just click ***OK*** to continue.
5. Click ***Options*** → ***Remote connection...*** and establish a remote connection as described in chapter 18.2.

Note that without a local license:

- TOPSPIN on the remote system must run with a licence.
- Local data cannot be accessed.

18.4 Security of Remote Connections

All data transferred during a remote control session is, by default, encrypted. This ensures that nobody can see data or commands by observing and recording your network traffic. TOPSPIN uses the Secure Socket Layer (SSL) technology for encryption, which is also used for secure web sites. SSL needs digital certificates on both sides of a connection to achieve a valid authentication. After a TOPSPIN installation, default certificate files are provided to secured connections. There is a chance, however small, such connections are attacked by a malicious person who also has the same default certificate files. If, for this reason, you want to create your own set of certificate files, you can do this by executing a script that is installed in `<tshome>/prog/server/make_new_certificates` and follow the instructions given there. To start a remote connection, the new certificate files must be installed on BOTH machines.

18.5 How to Access ICON-NMR from a Remote Web Browser

In TOPSPIN 1.3 and newer, ICON-NMR is web-enabled. The standard Bruker Automation Software now provides a built-in website which can be activated to allow remote access to ICON-NMR from any web browser which is networked to the spectrometer workstation. Experiments may be cancelled/submitted, the run may be paused or halted and spectra in PDF format are available from the browser window. No added software apart from ICON-NMR is required and configuration is performed via the standard ICON-NMR Configuration window. For security a SSL/HTTPS connection is supported. Pocket PC Internet Explorer is also supported for full spectrometer control via Windows Mobile 2003 (TM) or equivalent. PDF files of spectra may also be viewed on this platform making the mobile pocket spectrometer a reality.

The configuration of ICON-NMR web interface is described in the ICON-NMR manual, accessible ***Help*** → ***Manuals*** → [**Automation and Plotting**] ***IconNmr Automation Interface***. Note that ICON-NMR remote control does not require and is fully independent of TOPSPIN remote control.

Chapter 19

User Preferences

19.1 User Preferences

TOPSPIN can be tailored to your preference in many respects. This ranges from start-tup options to spectrum objects, menu settings, remote connections etc. Every standard user can create his/her own set of preferences.

To set user preferences:

- Click ***Options*** → ***Preferences*** [**`set`**]

A dialog box will appear with, at the left side, the categories that can be tailored

(see Fig. 19.1)

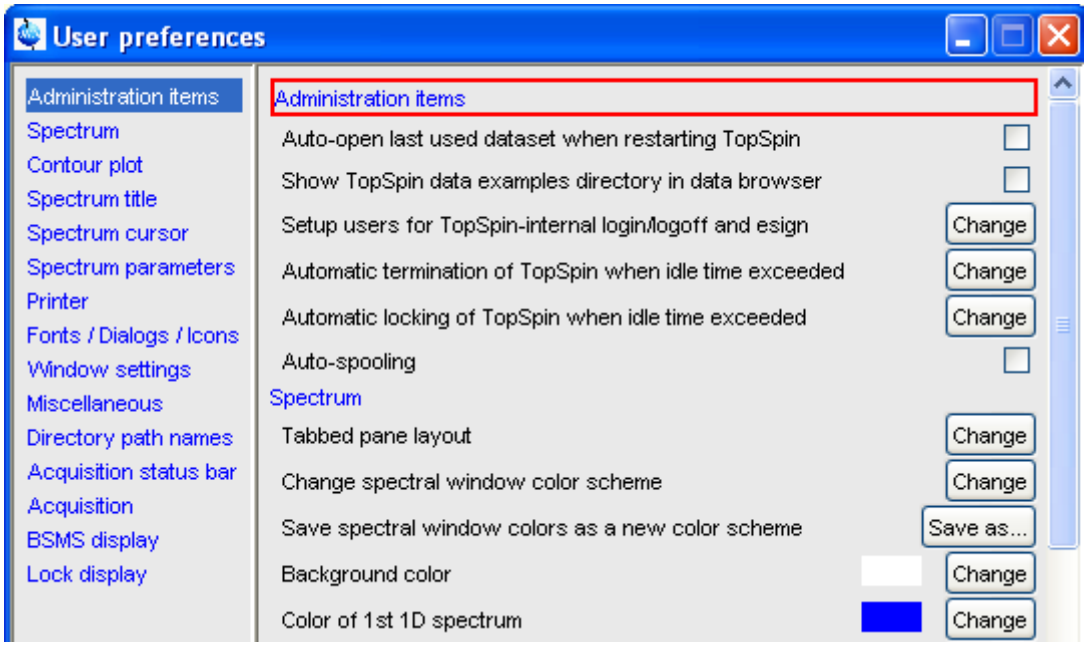


Figure 19.1

Click the cathegory of which you want to view/change certain objects. It will become highlighted and the corresponding objects will be displayed at the right part of the dialog box. For example, if you click *Spectrum*, the spectrum objects will appear at the top of the dialog box. The rest of this paragraph will describe some examples of setting various user preferences.

19.1.1 Define User Preferences Location for all Users

User Preferences are, by default, stored in the current users home directory:

<userhome>/.topspin-<hostname>

During the first TOPSPIN session, files with default settings are created there. They can then be modified with the ***set*** command and used in later sessions.

You can, however, also store user preferences at one central location, which are then used by all users. This location can even be a remote drive allowing you to use the same preferences on all computers in the network.

To do that:

1. Make a backup copy of the file `<tshome>/javaenv.cmd`.
2. Open the file `<tshome>/javaenv.cmd` using a text editor.
3. Locate the line "set SYSTEM_PROPS=-DXWINNMRHOME="%XWIN-NMRHOME%" -DCOMPUTERNAME=%COMPUTE....." near the beginning of the file.
4. Append a white space character and then:
   -DPROPDIR=<dir>
   to the end of this line, where <dir> is the definition of the storage directory, consisting of one or more parts (see below)
5. Close the editor.

The definition of the storage directory for User Preferences can take three forms:

-DPROPDIR=<mydir>

Stores the user properties in <mydir>/prop

Example: -DPROPDIR="/x y z" [1]

-DPROPDIR=<mydir> USER [2]

Stores the user properties in <mydir>/<login id>/prop, where <login id> is the id under which the user is logged into the operating system

Example: -DPROPDIR="/x y z USER" [1]

-DPROPDIR=CURDIR

Stores the user properties in <tshome>/prog/curdir/<login id>/prop, where <login id> is the id under which the user logged into the operating system

Please note that the specified directory must writable for all TOPSPIN users.

19.1.2 TOPSPIN Startup Actions

How to Open the Last Used Dataset on Startup

1. Click ***Options*** → ***Preferences*** [`set`].

---

1. The double quotes are only required if the directory contains white spaces
2. Specify exactly 1 space between the pathname and the string USER

2. Check, under *Administration items,* the option :

   Auto-open last used data set

How to Define the Startup Actions

TOPSPIN allows you to define any commands to be executed automatically after startup. To do that:

1. Click ***Options*** → ***Administration*** → ***Edit Startup File***.
2. Enter the desired startup command(s), in the appearing editor, for example:

```
re exam1d_13C 1 1 c:\\bio guest
efp
apk
abs
```

The above lines would cause TOPSPIN to display the dataset:

C:/bio/data/guest/nmr/exam1d_13C/1/pdata/1

and execute the command ***efp***, ***apk*** and ***abs*** on it.

Note that you can use a single forward slash (/) or a double backslash (\\) as path separator.

Note that in TOPSPIN 2.1 and newer, the file `autostart.mac` is a regular Topspin macro. In older versions, however, the file `autostart.prop` was used with a different format.

How to Define Auto-Termination after Idle Time

TOPSPIN can be configured to be terminated after a user specified idle time. To do that:

1. Click ***Options*** → ***Preferences*** [***set***].
2. Click the ***Change*** button to the right of the object

   Automatic termination of TOPSPIN when idle time has exceeded

   enter the NMR Administration password as requested and enter the number of minutes of allowed idle time.
3. Click ***OK*** to close the dialog, click ***OK*** to close the Preferences dialog.
4. Restart TOPSPIN to activate the change.

If the user does not execute any commands (from the command line, menu or tool buttons), a dialog will appear with an ***OK*** button (to terminate immediately) and/or ***Cancel*** button (to continue).

Automatic termination frees the license used by this TOPSPIN instance for other users. This solves the problem of users leaving TOPSPIN open and blocking a floating license although they do not currently use it.

How to Define Auto-Locking after Idle Time

TOPSPIN can be configured to lock the interface after a user specified idle time. To do that:

1. Click ***Options*** → ***Preferences*** [`set`].
2. Click the ***Change*** button to the right of the object

   Automatic locking of TOPSPIN when idle time has exceeded

   enter the NMR Administration password as requested and enter the number of minutes of allowed idle time.
3. Click ***OK*** to close the dialog, click ***OK*** to close the Preferences dialog.

If the user does not any commands (from the command line, menu or tool buttons), the TOPSPIN interface will be locked (see Fig. 19.2).

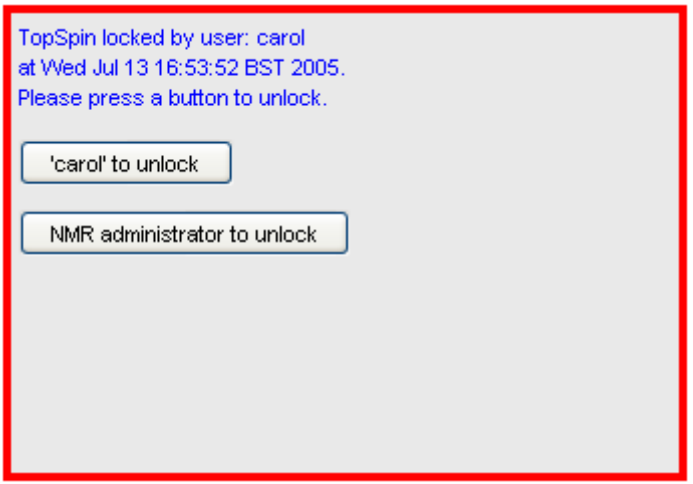
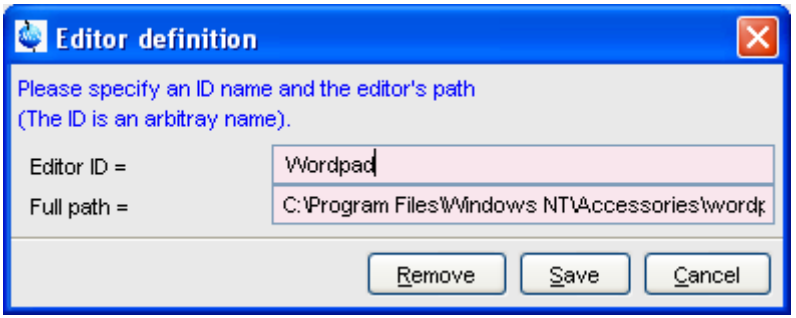

TopSpin locked by user: carol
at Wed Jul 13 16:53:52 BST 2005.
Please press a button to unlock.
'carol' to unlock
NMR administrator to unlock

Figure 19.2

How to Change the Preferred Editor

You can choose your preferred editor as it is used by commands like ***edau***, ***edpul***, ***edcpd*** etc. To do that:

1. Click ***Options*** → ***Preferences*** [***set***].
2. Click ***Miscellaneous*** in the left part of the dialog box.
3. Click the ***Change*** button to the right of the object *Preferred text editor* enter the desired Editor and its path. For example for Wordpad under Windows 2000/XP, this would look like:



4. Click ***Save*** to save the changes.

If no editor is specified here, the TOPSPIN internal editor is used. It the file being edited is read-only, the TOPSPIN internal viewer is used.

How to Configure the Tab Bar

The default Tab bar at the top of the data window consist of Tabs to switch between various dataset objects like *Spectrum*, *Parameters*, *Title*, etc. You can, however, configure the Tab bar to contain Tabs for interactive data manipulation like *phase correction*, *integration* etc. These Tabs have the same function as the corresponding buttons in the upper tool bar (see chapter 11 and 12) but are easier to access. You can configure the Tab bar as follows:

1. Click ***Options*** → ***Preferences***
2. Click ***Spectrum*** in the left part of the *User preferences* box.
3. Click the ***Change*** button to the right of the object *Tabbed pane layout.*
4. Check the desired Tabs, uncheck the others.
5. Click ***OK***

How to Configure the Right-click Menu Function

Right-clicking a pull-down or popup menu, can perform various actions. This can be configured as follows:

1. Right-click an empty part of the menubar and choose ***Define Right-Click Action*** from the popup menu.

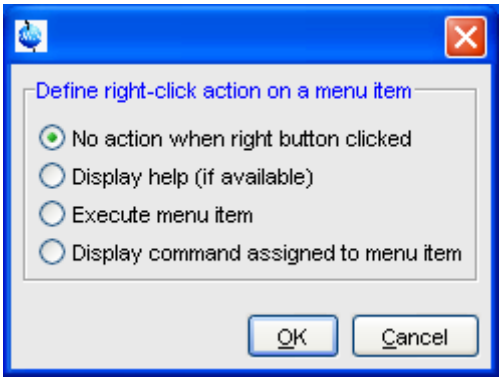

Define right-click action on a menu item
No action when right button clicked
Display help (if available)
Execute menu item
Display command assigned to menu item
OK
Cancel

Figure 19.3

2. In the appearing dialog (see Fig. 19.3), select the desired action.
3. Click ***OK***

19.1.3 Changing Colors

How to Change Colors of Data Objects on the Screen

The color of various objects in a data window on the screen, like 1st, 2nd and 3rd spectrum, axis, parameters etc. can be changed. To set these colors:

1. Click ***Options*** → ***Preferences*** [**`set`**].
2. Click ***Spectrum*** in the left part of the *User preferences* box.
3. Click the ***Change*** button to the right of the object you want to change e.g.:



4. Select the desired color in the appearing dialog box and click ***OK***
5. Click ***Apply***

How to Change Colors of Data Objects on the Printer

The color of data objects on the printer is independent from the color of the corresponding object on the screen. To set print colors:

1. Click ***Options*** → ***Preferences*** [**`set`**].
2. Click ***Printer*** in the left part of the *User Preferences* box.
3. Click the ***Change*** button to the right of the object you want to change, e.g.:



4. Select the desired color in the appearing dialog box and click ***OK***
5. Click ***Apply***

How to Change Colors of the Lock Display

The colors of lock display objects can be changed as follows:

1. Click ***Options*** → ***Preferences*** [**`set`**].
2. Click ***Lock display*** in the left part of the *User preferences* box.
3. Click the ***Change*** button to the right of the object you want to change, e.g.:



4. Select the desired color in the appearing dialog box and click ***OK***
5. Click ***Apply***

How to Create a New Data Window Color Scheme

To create a new data window color scheme:

1. Click ***Options*** → ***Preferences*** [**`set`**].
2. Change any color of the objects *Spectrum, Spectrum title, Spectrum cursor or Spectrum parameters*.
3. Click ***Apply***
4. Click ***Spectrum*** in the left part of the *User preferences* box.
5. Click the button ***Save as...*** to the right of the object:

Save spectral window colors as a new color scheme

and enter a new name in the appearing dialog box.

6. Click ***OK***

How to Read a Different Data Window Color Scheme

1. Click ***Options*** → ***Preferences*** [`set`].
2. Click ***Spectrum*** in the left part of the *User preferences* box.
3. Click in the list box to the right of the object:

   Change spectral window color scheme

   and select an element from the appearing list.
4. Click ***OK***

TOPSPIN is delivered wit two colors schemes:

- *light* (default): a white background with black axes
- *dark*: a dark blue background with a white axes

How to Change Peak and Integral table Colour/Spacings

1. Click ***Options*** → ***Preferences*** [`set`].
2. Click ***Miscellaneous*** in the left part of the *User preferences* box.
3. Click in the list box to the right of the object:

   Table colors (see Fig. 19.4)

   for simple tables like peaks, solvents, nuclei tables

   Tree table colors

for nested lists like the integral table.

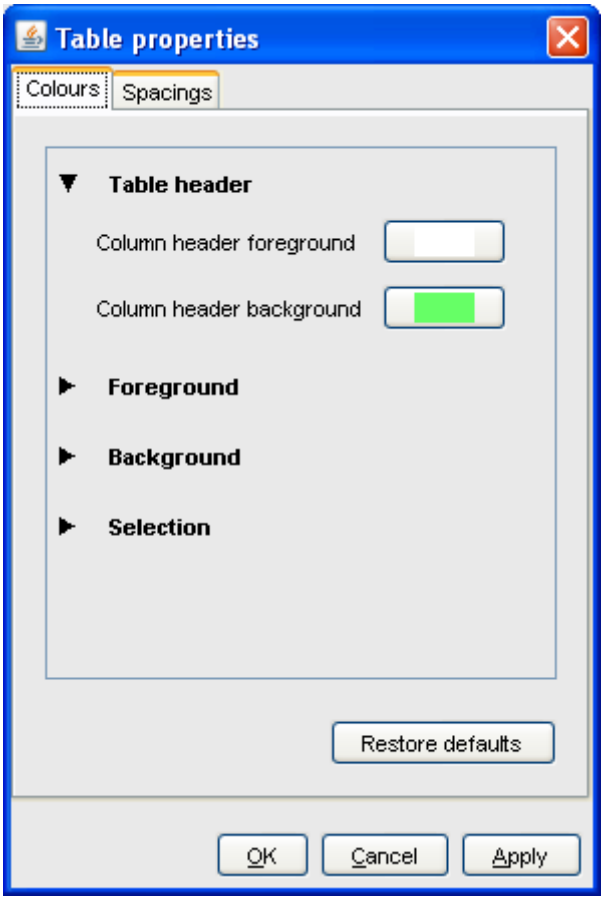


Figure 19.4

Set the desired colours and spacings.

4. Click ***OK***

Note that table colours and spacings can also be change from a table. To do that, right-click any table entry and choose ***Table properties...***

19.1.4 Changing Lines

How to Create Thick Lines on the Screen

To create thick (double width) lines for high resolution display or screendumps:

1. Click ***Options*** → ***Preferences*** [`set`].
2. Click ***Spectrum*** in the left part of the dialog box.
3. Enable the entry ***Use thick lines***
4. Click ***OK***

How to Create Thick Lines on the Printer

To create thick (double width) lines for high resolution display or screendumps:

1. Click ***Options*** → ***Preferences*** [`set`].
2. Click ***Printer*** in the left part of the dialog box.
3. Enable the entry ***Use thick lines***
4. Click ***OK***

19.1.5 Changing Fonts

How to Change All Fonts of the Topspin Interface

1. Click ***Options*** → ***Preferences*** [`set`].
2. Click ***Fonts/Dialogs/Icons*** in the left part of the dialog box.
3. Set the entry *Change size fonts listed above by .... points*
   You can enter a positive or negative number.

Fig. 19.5 shows an example of increasing the font sizes by 4 points.



Figure 19.5

4. Click ***OK*** to store the new value.



Figure 19.6

Fig. 19.6 shows the same part of the Preferences dialog box dialog box after the change of fonts. Note that:

- The value all four font entries has been increased by 4.
- The font of the dialog box itself is larger.
- The change size has been reset to 0.

How to Change the Font of the TOPSPIN menu

To change the font of the TOPSPIN menu:

1. Click ***Options*** → ***Preferences*** [`set`].

2. Click ***Fonts/Dialogs/Icons*** in the left part of the dialog box.
3. Click the ***Change*** button to the right of the *Menu font* object:



4. Select the desired *name*, *style* and/or *size* in the appearing dialog box.
5. Click ***OK*** to store the new font.
6. Click ***Apply***

The default menu font is *Dialog/Plain/18* and looks like this:



After changing the font to, for instance, to *Serif/Italic/18*, the menu looks like this:



A change in menu font also affects all sub-menus and popup menus.

How to Change the Font of the Tab bar

1. Click ***Options*** → ***Preferences*** [`set`].
2. Click ***Fonts/Dialogs/Icons*** in the left part of the dialog box.
3. Click the ***Change*** button to the right of the *Dialog window font* object.
4. Select the desired *name*, *style* and/or *size* in the appearing dialog box.
5. Click ***OK*** to store the new font.
6. Click ***Apply***

Fig. 19.7 and Fig. 19.8 shows a Tab bar with font size 10 and 14 respectively.

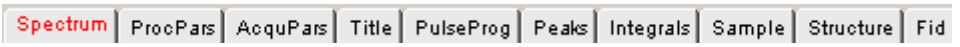


Figure 19.7 Tab bar with font size 10



Figure 19.8 Tab bar with font size 14

How to Change the Font of Dialog Boxes

1. Click ***Options*** → ***Preferences*** [***set***].
2. Click ***Fonts/Dialogs/Icons*** in the left part of the dialog box.
3. Click the ***Change*** button to the right of the *Dialog window font* object.
4. Select the desired *name*, *style* and/or *size* in the appearing dialog box.
5. Click ***OK*** to store the new font.
6. Click ***Apply***

Fig. 19.9 shows an example of a dialog box with the font *Times New Roman Italic*

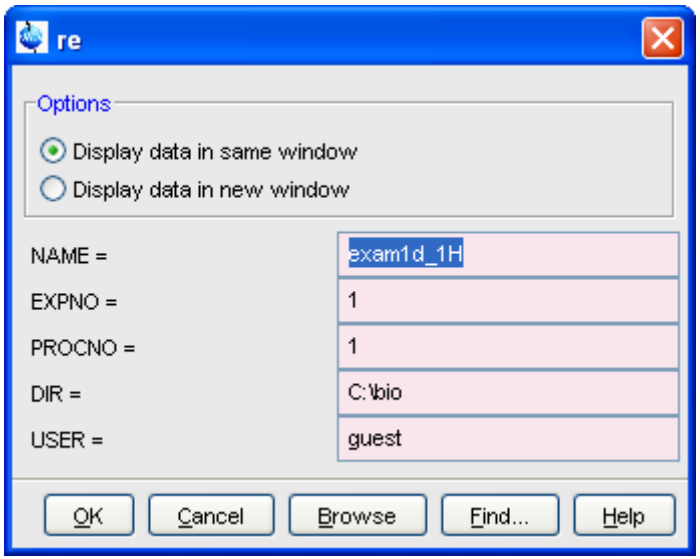


Figure 19.9

How to Change the Font of the Browser

To change the font of the browser:

1. Click ***Options*** → ***Preferences*** [***set***].

2. Click ***Fonts/Dialogs/Icons*** in the left part of the dialog box.
3. Click the ***Change*** button to the right of the *Dialog window font* object.
4. Select the desired *name*, *style* and/or *size* in the appearing dialog box.
5. Click ***OK*** to store the new font.
6. Click ***Apply***

TOPSPIN must be restarted for this change to become effective. Note that this change will affect all dialog boxes.

How to Change the Font of the Command Line

1. Click ***Options*** → ***Preferences*** [`set`].
2. Click ***Fonts/Dialogs/Icons*** in the left part of the dialog box.
3. Click the ***Change*** button to the right of the *Command line font* object.
4. Select the desired *name*, *style* and/or *size* in the appearing dialog box.
5. Click ***OK*** to store the new font.
6. Click ***Apply***

How to Change the Font of the Status Line

1. Click ***Options*** → ***Preferences*** [`set`].
2. Click ***Fonts/Dialogs/Icons*** in the left part of the dialog box.
3. Click the ***Change*** button to the right of the *Status line font* object.
4. Select the desired *name*, *style* and/or *size* in the appearing dialog box.
5. Click ***OK*** to store the new font.
6. Click ***Apply***

19.1.6 Changing Acquisition settings

How to Auto-Archive existing expnos

1. Click ***Options*** → ***Preferences*** [`set`].
2. Click ***Acquisition*** in the left part of the dialog box.
3. Click the Change button to the right of the item *Configure Accounting & Data Archiving after 'zg'* (see Fig. 19.10).
4. In the appearing dialog (see Fig. 19.11), configure archiving as described in

the dialog.

5. Click ***OK***.

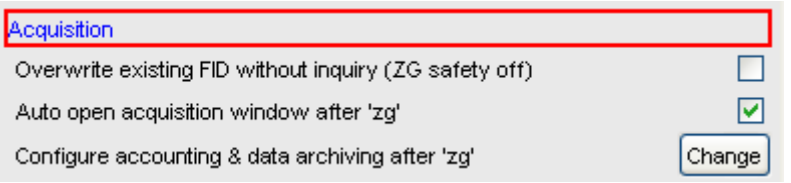

Acquisition
Overwrite existing FID without inquiry (ZG safety off)
Auto open acquisition window after 'zg'
Configure accounting & data archiving after 'zg'
Change

Figure 19.10

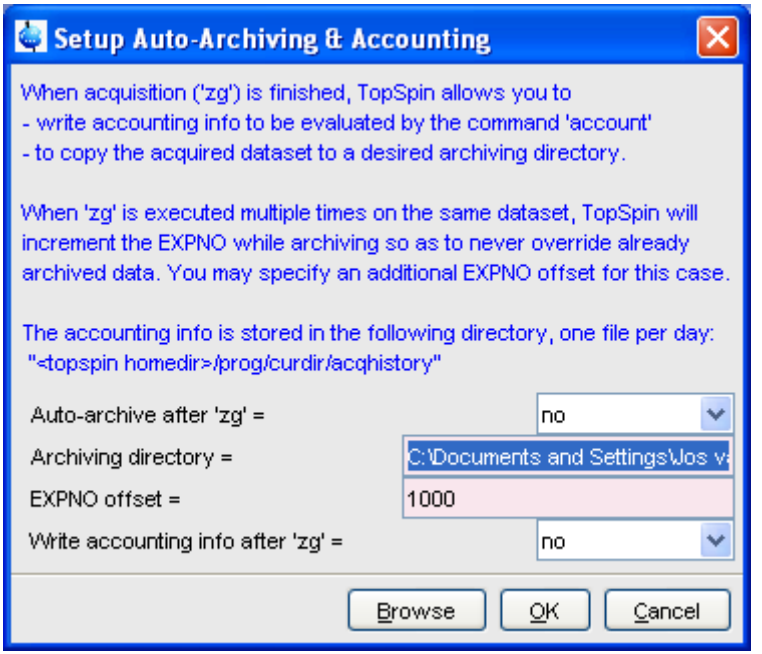

Setup Auto-Archiving & Accounting
When acquisition ('zg') is finished, TopSpin allows you to
- write accounting info to be evaluated by the command 'account'
- to copy the acquired dataset to a desired archiving directory.
When 'zg' is executed multiple times on the same dataset, TopSpin will increment the EXPNO while archiving so as to never override already archived data. You may specify an additional EXPNO offset for this case.
The accounting info is stored in the following directory, one file per day:
"<topspin homedir>/prog/curdir/acqhistory"
Auto-archive after 'zg' =
no
Archiving directory =
C:\Documents and Settings\Jos
EXPNO offset =
1000
Write accounting info after 'zg' =
no
Browse
OK
Cancel

Figure 19.11

19.2 Command Line Preferences

How to Resize the Command Line

By default, the TOPSPIN command line shows one command, the command that is

currently entered, e.g.:



However, you can resize the command line to show the currently entered command plus the last and second last command, e.g.:



You can toggle between the two different command line sizes as follows:

- Click ***View*** → ***Resize command line***

or

- Right-click in the command line and click ***Resize command line***

How to Set the Minimum and Maximum Command Line Size

By default, the size of the command line can be toggled between 1 and 3. You can, however, change this minimum and maximum value, respectively. To do that:

1. Click ***Options*** → ***Preferences*** [`set`].
2. Click ***Fonts/Dialogs/Icons*** in the left part of the dialog box.
3. Specify the *Minimum visible command lines* (> 0).
4. Specify the *Maximum visible command lines* (≥ *Minimum visible*).
5. Click ***Apply***

19.3 Disabling/Enabling Toolbar Buttons, Menus and Commands

How to Hide the Upper and Lower Toolbars

Right-click in an empty area of one of the toolbars and choose:

Hide the toolbars

from the appearing popup menu (see Fig. 19.12).

To restore the toolbars:

☞ press the keys SHIFT+ESC

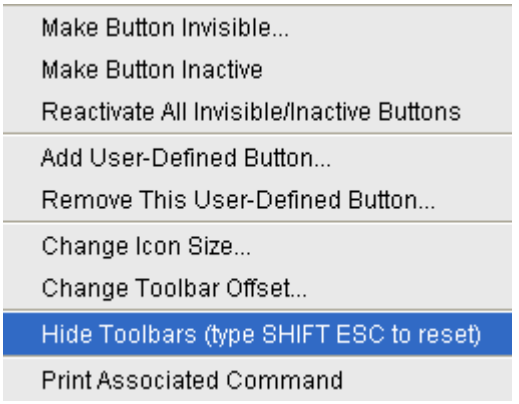


Figure 19.12

How to Hide the Menubar

Right-click in an empty area of the Menubar and choose:

Hide the menubar

from the appearing popup menu.

To restore the menubar:

☞ press the keys SHIFT+ESC

How to Disable/Remove Toolbar Buttons

Buttons of the upper or lower toolbar can be disabled or removed as follows:

1. Right-click a toolbar button.
2. Choose one of the entries:

   ☞ ***Make this button invisible*** to remove the button from the toolbar

   ☞ ***Make this button inactive*** to disable the button (it will appear greyed)

To restore the complete toolbars, click:

☞ ***Reactivate all invisible or inactive buttons*** to restore the default toolbar

How to Disable/Remove Menus or Commands

By default, all existing TOPSPIN commands can entered from the menu and/or from the command line. You can, however, selectively disable/remove commands or menus. This is typically done by system administrators who want to disable certain functions for standard users.

Open the Menu Configuration table as follows:

1. Click ***Options*** → ***Preferences*** [**`set`**].
2. Click ***Fonts/Dialogs/Icons*** in the left part of the dialog box.
3. Click the ***Change*** button of the entry *Disable/Enable menus and commands*.

The table consists of the following columns:

Command	Description	Menu	Status

You can disable/remove:

- *Menus*, e.g. ***Options***

  to be found in the column **Menu**
- *Sub-menus*, e.g. ***Options*** → ***Administration tools***

  to be found in the column **Menu**
- *Menu entries*, e.g. ***Options*** → ***Preferences***

  to be found in the column **Description**
- *Commands*, e.g. ***set***

  to be found in the column **Command**

Note that in this configuration table, each *menu entry* corresponds to a certain *command*. In the TOPSPIN menu, most commands are indicated in square brackets behind the corresponding menu entries, e.g.:

☞ ***Processing*** → ***Fourier transform*** [**`ftf`**]

Menu entries which are not used very often appear without the corresponding command indicated, e.g.:

☞ ***Options*** → ***Preferences***

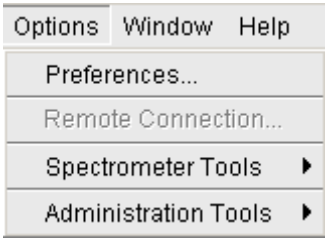
However, if you want, you can look up the corresponding command, in this case

set, in the configuration table and use it.

As an example, we will describe how you can disable/remove the *menu entry* ***Remote connection..*** in the ***Options*** menu:

1. Open the configuration table as described above.
2. Scroll to the *Description* ***Remote connection***
3. Set the *Status* to disabled.
4. Click ***Apply***

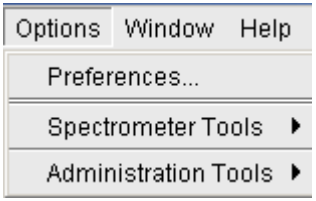
Clicking the TOPSPIN ***Options*** menu, will now show the following popup menu:



The entry ***Remote connection..*** is greyed and can no longer be used.

Go back to the Configuration table, change the *Status* of ***Remote connection...*** to invisible and click ***Apply***.

Clicking the TOPSPIN ***Options*** menu, will now show following popup menu:



The entry ***Remote connection..*** has disappeared.

Note that if you disable or remove a *menu entry*, the corresponding *command* is automatically disabled. For example, if you disable:

☞ ***Analysis*** → ***Deconvolution*** [***dcon***]

entering ***dcon*** on the command line will lead to an error message.

How to (Re)enable a disabled Command/Menu

1. Open the Menu Configuration table as described above.
2. Set the Status of a disabled or removed (invisible) entry to enabled.
3. Click ***OK*** to close the Configuration table.

How to (Re)enable All Commands/Menus

1. Open the Menu Configuration table as described above.
2. Click the ***Reset*** button to enable all menus and commands.
3. Click ***OK*** to confirm the appearing message.
4. Click the ***OK*** button to close the Configuration table.

19.4 Resizing/Shifting Toolbar Icons

How to Change the Toolbar Icon Size

1. Right-click of the toolbar,
2. In the appearing popup menu (see Fig. 19.13), click:

   ☞ ***Change Icon Size...***

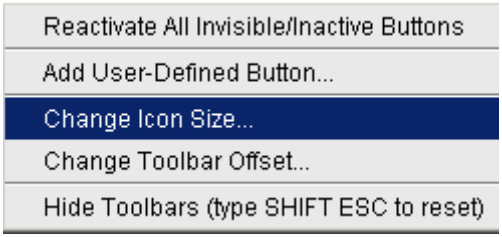

Reactivate All Invisible/Inactive Buttons
Add User-Defined Button...
Change Icon Size...
Change Toolbar Offset...
Hide Toolbars (type SHIFT ESC to reset)

Figure 19.13

3. Enter the icon size in the appearing dialog and click ***OK***.

How to Shift Toolbar Icons to the Right

1. Right-click at an empty area of the toolbar.
2. In the appearing popup menu (see Fig. 19.13), click:

   ☞ ***Change Toolbar Offset...***

3. Enter the toolbar offset in the appearing dialog and click ***OK***.
4.

19.5 Defining Source Directory for Programs/Lists etc.

TOPSPIN 2.1 and newer allow you to defined the source directories for pulse programs, AU programs, integral ranges, various lists etc. In TOPSPIN 2.0 and older, the source directory for these items was fixed: <tshome>/exp/stan/nmr. Now you can define a individual source directories for each item. To do that:

1. Open the dialog of any of the items, e.g. with the command ***edau***, ***edlist*** or ***edmisc***.
2. Click ***Options*** → ***Manage Source Directories***

   A dialog will appear showing a list of items with the current source directo-

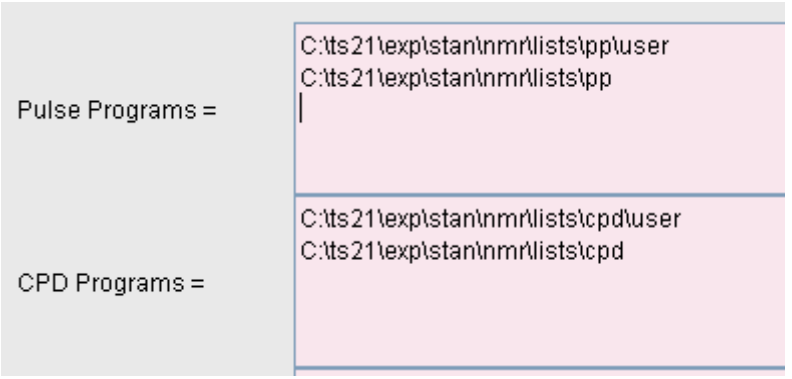


Figure 19.14

ries. By default, two source directories are present, one for user defined items and one for Bruker items. This list can be modified or extended with your preferred source directories, e.g.:

C:\my-pulse-programs\
C:\ts21\exp\stan\nmr\lists\pp\user
C:\ts21\exp\stan\nmr\lists\pp

You can do this for each item separately. Items will be searched for in the order of the directories specified.

Chapter 20

User Extensions

TOPSPIN offers various ways to extend the standard commands, buttons, programs etc.

20.1 User Notebook

You can create your own user specific notebook with the command:

☞ ***View*** → ***Notebook*** [`nbook`]

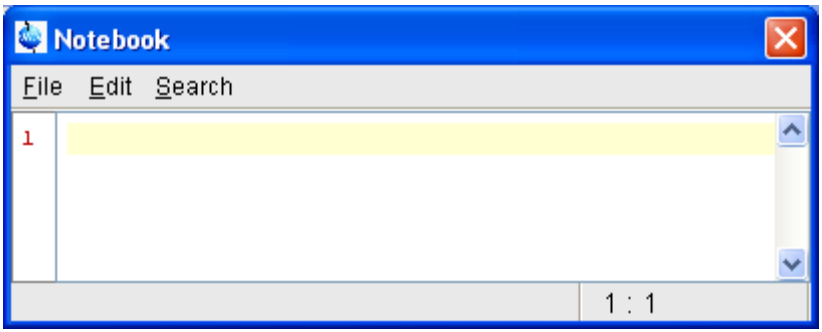


Figure 20.1

This can be used to store and retrieve any personal notes, information etc.

20.2 Macros

A macro contains a sequence of TOPSPIN commands. It can be created with the command ***edmac***. A simple macro for processing and plotting the current dataset is:

```
em
ft
apk
sref
autoplot
```

All entries in a macro file must be written in lower case letters.

In TOPSPIN 1.3 and newer, a macro may contain Python commands. Any line in a macro that starts with:

```
py>
```

executes a Python command. An example of such a macro is:

```
re exam1d_13C 1 1 C:\bio guest
efp
py>NEWWIN() # open new window
re exam1d_1H 1 1 C:\bio guest
efp
py>x = INPUT_DIALOG()
py>if x == None: EXIT()
py>y = 2* int(x[0])
py>MSG("done: y=" + str(y))
```

Note that commands like `NEWWIN()`, `INPUT_DIALOG()`, `MSG()` and `EXIT()` are Bruker defined whereas "`x=`" and "`if`" are original Python commands.

Once created, a macro can be executed by entering its name on the command line.

20.3 AU Programs

An AU program may contain TOPSPIN commands, AU macros and C-language statements. It can be created with the command ***edau***. A simple AU program which performs the ***efp*** command on a series of dataset *expno*'s is:

```
#include <lib/util.h>
```

```
int first, max;
char string[80];

first = expno;
GETINT ("Enter first expno to process : ",first)
max = 10;
GETINT ("Enter number of expnos : ",max)
WPAR("tmpmefp","proc")
expno = first;
TIMES(max)
RPAR("tmpmefp","proc")
EFP
IEXPNO
END
DEXPNO
DELPAR("tmpmefp")
QUITMSG("--- multiefp finished ---")
```

Note that TOPSPIN commands like EFP and RPAR and AU macros like IEXPNO are written in upper case letters whereas C-language statements like are written in lowercase letters. Once created, an AU program can be executed by entering its name on the command line.

For more information on writing AU programs:

☞ Click ***Help*** → ***Manuals*** → [**Programming Manuals**] ***AU programming***

20.4 Python Programs

A Python program may contain TOPSPIN commands, User Interface functions and Graphic functions. It is created with ***edpy***.

The Python program below reads a region of the real part of a spectrum and the corresponding region of the imaginary part and displays both. The simplest form of DISPLAY_DATALIST is used.

```
from TopCmds import *
import math
region = [80, 72] # define region in ppm
# open testdata, don't display
testdata = ["exam1d_13C", "1", "1", "c:/Bruker/topspin", "guest"]
```

```
RE(testdata, "n")
# read real and imaginary points of the region
reals = GETPROCDATA(region[0], region[1])
imags = GETPROCDATA(region[0], region[1], data-
const.PROCDATA_IMAG)
if reals == None or imags == None: EXIT()
# set up list of data to be displayed and respective axis info list
dataList = [reals, imags]
# display the data in the list
DISPLAY_DATALIST(dataList)
```

For more information on writing Python program:

☞ Click ***Help*** → ***Manuals*** → [**Programming Manuals**] ***Python programming***

20.5 Button Panels

A button panel is a window with user-defined buttons for executing TOPSPIN commands, AU programs, Python programs or macros. It appears as an integral part of the active data window and acts on that. Bruker delivers a few standard button panels like ***bnmr*** and ***bnmrsel***. To create your own button panels, you can modify one of these or write them from scratch.

In this description we will create a very simple button panel with some 1D processing commands and print/export buttons (see Fig. 20.2)

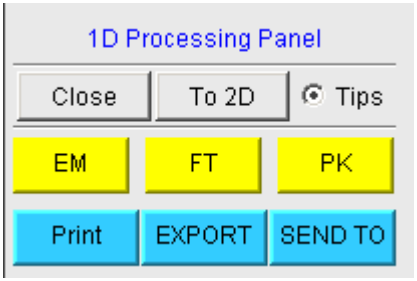


Figure 20.2

To write this button panel, take the following steps:

1. Open the Windows Explorer and navigate to the subdirectory

   `userdefined`

of the users properties directory [1].

2. Create a text file with the name

   `cmdpanel_<name>.prop`

   where <name> is the name of the button panel.

3. Enter the button definitions including *Panel title*, *Colors*, *Toggle buttons*, *Top buttons*, *Panel layout*, *Panel buttons* and *Tooltips*.

4. Save the file under a name `cmdpanel_<xxx>.prop`

   where `<xxx>` is the actual name of your command panel.

   Make sure the extension of the file is `.prop` and not `.txt`, `.prop.txt` or anything else.

5. Enter ***bpan <xxx>*** on the command line to open the button panel.

Here is an example for a small button panel for 1D processing:

```
# Color definitions used in this file (RGB)

BLUE1=51$ 204$ 255
YELLOW1=255$ 255$ 0
GREEN1=84$ 196$ 20

# Title definition

TITLE=1D Processing Panel
TITLE_COLOR=0$ 0$ 255

# Toggle button definition

TOGGLE_BUTTON=To 2D
TOGGLE_CMD=bpan bproc2d
TOGGLE_TIP=Switch to 2D processing

# Top row button definition

TOP_BUTTONS=EM$ $FT$ $PK$ $
TOP_COLORS=YELLOW1$ YELLOW1$ YELLOW1
TOP_CMDS=em$ ft$ pk
TOP_TIPS=Exponential multiplication $\
Fourier transform$\
Phase correction
```

1. To locate this, enter ***hist*** and look for the entry "User properties directory=".

```
# Panel button definitions

# LAYOUT format: rows columns hgap vgap
PAN_LAYOUT=1$ 3$ 8$ 8

PAN_BUTTONS=Print$ $ EXPORT$ $SEND TO$ $
PAN_COLORS=BLUE1$ BLUE1$ BLUE1
PAN_CMDS=prnt$ exportfile$ smail
PAN_TIPS=Print the spectrum<br>\
as it appears on the screen$\
Export the dataset<br>\
to png, jpg, bmp etc.$\
Send the dataset by email
```

If you type ***bpan exam***, a panel with 75 buttons will appear: 5 rows and 15 columns. The corresponding panel file is called `cmdpanel_exam.prop`, which resides in the directory:

<tshome>/classes/prop/English

In the same directory, you can find the files `cmdpanel_bnmr.prop` and `cmdpanel_bnmrsel.prop`, which are used to display the *bnmr* and *bnmrsel* panels described above.

The texts displayed on the buttons can be graphically adjusted in various ways, because the text may optionally be specified in html format. In the example above, the PAN_BUTTONS property has no html tags, therefore the texts are displayed in black using the default TOPSPIN *Dialog window font* as specified in the User Preferences (command ***set***). If you replace the text `Print` by the following:

```
<html><font size=10><font
color=\"00BF00\">Print<br>Now</font></html>
```

then the new text "Print Now" is displayed in green (the color to be specified in RGB hex code), with 10 points font size. Also, "Now" is display below "Print" due to the html
 (= break line) tag.

Note that:

- The *Close* button and *Tips* switch are automatically created. You don’t need to specify them.
- The TOGGLE button is typically, but not necessarily, used to call another button panel. In this example it calls the panel ***bproc2d***. If TOGGLE_BUTTON is specified without a value, i.e. the entry is

"TOGGLE_BUTTON=" instead of "TOGGLE_BUTTON=action text", the corresponding button is not shown in the panel.

- Items must be separated with the "$" character, button items with "$ $"
- A "\" followed by "end of line" continues an item on the next line.
- Tooltips may use html tags for text formatting.
- Commands may be specified as single commands like "em" or as composite commands like "em\nft\npk". Note that in the latter case, the commands must be separated by "\n".
- When the ***bpan <name>*** command comes up with an error message, carefully check the syntax of your cmdpanel file. A common mistake is to specify the button items incorrectly. With the keyword PAN_LAYOUT you define the number of rows and columns, and the number of items will become rows*cols. All specifications such as PAN_BUTTONS, PAN_COLORS, etc. must have this number of members, otherwise you will get some kind of TOPSPIN error. Please insert the "$" separator to make sure the item count is correct.

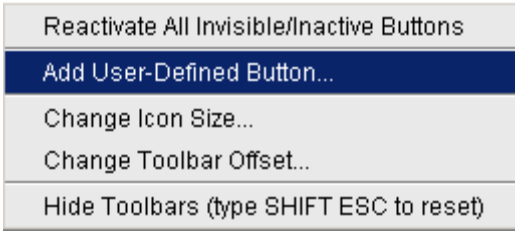
20.6 Adding User Defined Buttons to the Toolbars

The upper and lower toolbar at the top of the TOPSPIN window can be extended with user defined buttons. They can be assigned to any TOPSPIN command, macro, AU program or Python program.

To create a user defined button, take the following steps:

1. Right-click at an empty area of the toolbar.
2. In the appearing popup menu, click:

   Add User-Defined Button


Reactivate All Invisible/Inactive Buttons
Add User-Defined Button...
Change Icon Size...
Change Toolbar Offset...
Hide Toolbars (type SHIFT ESC to reset)

3. In the appearing dialog box (see Fig. 20.3)

a) Choose between the options *text label* or *icon*
The corresponding parameters are enable/disabled.

b) Enter the *command name*, the *tool tip* and the *label text* or *icon file* pathname.

c) For a text label: set its *font*, *text color* and *background color.*

d) For an icon label: specify the icon image filename

e) Set the *separator* flag to *yes* or *no* and select the data *dimension*(s) for which the button must appear.

For an icon label, you must stored the icon image file in one of the following directories:

- <*user-home*>/.topspin-<hostname>/prop/userdefined (only available for this user)
- <tshome>/classes/prop (available for any user)
- any directory (the full pathname must be specified in the icon label field)

The formats `.gif`, `.jpg`, `.jpeg` and `.png`, are supported. Standard TOPSPIN toolbar icons have a size of 16 * 16 pixels. If your own icons have a different size, they are automatically rescaled and displayed at the standard size.

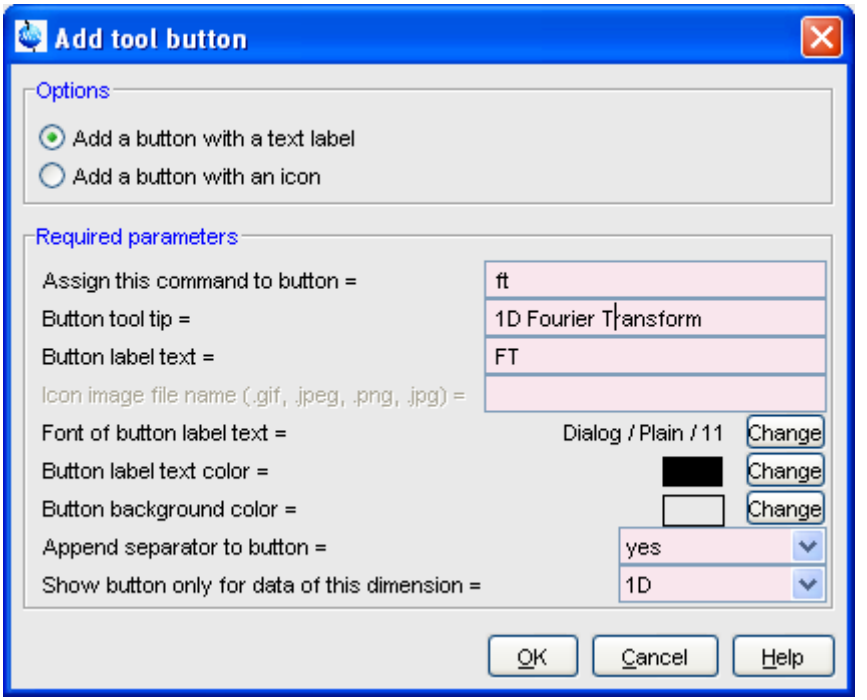


Figure 20.3

In the example above, a button **FT** is created with a separator, which only appears for 1D datasets, and executes the command ***ft***.

How do I Remove a User Defined Toolbar Button

Right-click the toolbar button and click:

Remove this user-defined button...

in the appearing popup menu (see Fig. 20.4).

How do I Shift a User Defined Toolbar Button to the left/right

Right-click the toolbar button and click:

Shift left

or

Shift right

in the appearing popup menu (see Fig. 20.4).

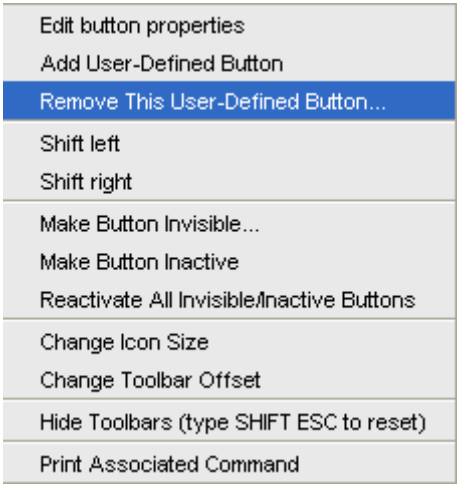


Figure 20.4

The button definitions are stored in the file `toolbar_user.prop` which resides in the subdirectory `userdefined` of the user properties directory. To locate this directory enter the TOPSPIN command ***`hist.`*** A dialog box will show the contents of the `history` file. Near the top of this file, you will see an entry "User properties directory=".

For icon image buttons, the formats `.gif`, `.jpg`, `.jpeg` and `.png`, are supported. Standard TOPSPIN toolbar icons have a size of 16 * 16 pixels. If your own icons have a different size, they are automatically rescaled and displayed at the standard size.

20.7 Adding User Defined Menus to the Menubar

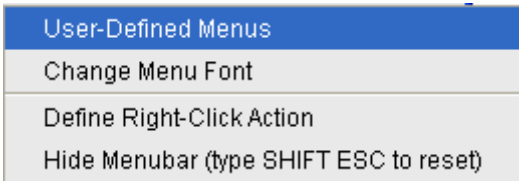
The menubar at the top of the TOPSPIN window can be extended with user defined menus. They can be assigned to any TOPSPIN command, macro, AU program or Python program. They are specific for the dimensionality of the active dataset.

To create a user defined menu, take the following steps:

1. Open a dataset of the desired dimensionality.
2. Right-click at an empty area of the menubar.

3. In the appearing popup menu, click:

   User_defined Menus



4. In the appearing dialog box (see Fig. 20.5).
   a) Click ***Add Menu*** and specify the **Menu Name** in the appearing dialog.
   b) Click ***Add Menu Item*** and specify the **Menu Item** name and the corresponding **Command** in the appearing dialog.
   c) Click ***Apply***.

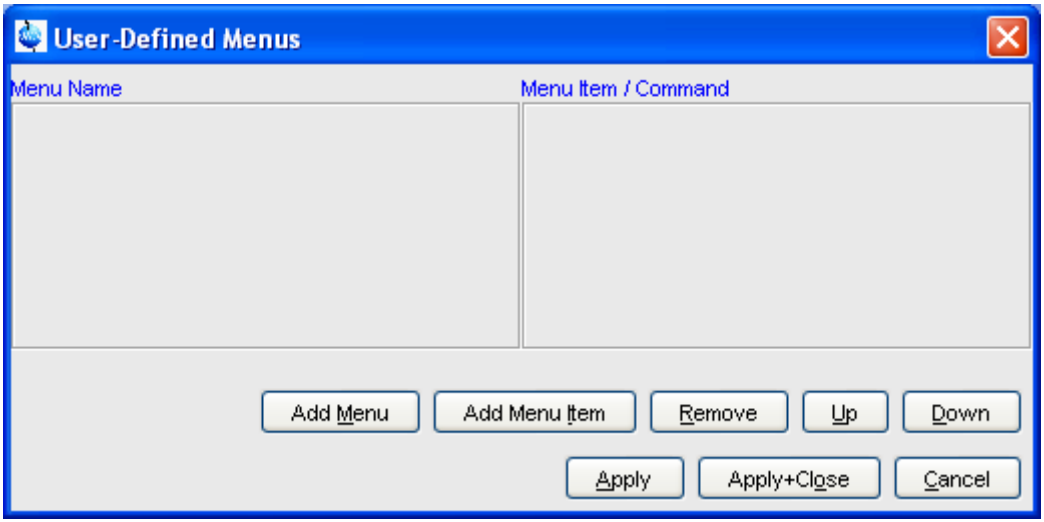


Figure 20.5

The new menu will appear in the menubar.

Furthermore the dialog box in Fig. 20.5 contains the following buttons:

- ***Remove*** : Remove menu names and/or menu items
- ***Apply+Close*** : Apply any changes and close the dialog box
- ***Up/Down*** : Move up/down the menu name list

- ***Cancel*** : Close the dialog box discarding any changes.

User defined menu definitions are stored in the file `umbar_menubar1d.prop`, `umbar_menubar2d.prop` or `umbar_menubar3d.prop` depending on the data dimensionality. These files resides in the subdirectory `userdefined` of the user properties directory. To locate this directory enter the TOPSPIN command ***hist.***

20.8 Adding User Defined Guides

TOPSPIN offers several guides like the Acquisition Guide (command ***aqguide***), the Processing Guide (command ***prguide***) and the T1/T2 Guide (command ***t1guide***). You can set up your own guides, which can be adaptations of Bruker guides or new written ones. In order to do that, you must edit the file `toolbar_user.prop` and `cmdtab_user.prop` in the directory:

<user properties directory>/userdefined/

To identify this directory, enter the command ***hist*** in TOPSPIN.

The file `toolbar_user.prop` contains the guide definition. If the file does not exist, it must be created. Here is an example of a user-modified T1/T2 guide.

```
MyT1T2Toolbar=\
NM=t1fid_40.gif, NM2=$Extract fid, TIP=$Do rser,
CMD=_t1_fid, END=,\
NM=t1spec_40.gif, NM2=$Transform, TIP=$Do ef+apk,
CMD=_t1_spec, END=,\
NM=t1ranges_40.gif, NM2=$Ranges, TIP=$Enter integ. mode,
CMD=_t1_ranges, END=,\
NM=t1screen_40.gif, NM2=$Relax. Window, TIP=$Enter Relax
mode, CMD=_t1_relax, END=,\
NM=-, END=,\
NM=myicon.gif, NM2=$Fit Methods, TIP=$Select fit funcs.,
CMD=_t1_func, END=,\
NM=c:/myicons/myicon1.gif, NM2=$Start, TIP=$ct1,ct2, sim-
fit, CMD=_t1_start, END=,\
NM=c:/myicons/myicon2.gif, NM2=$Show Report, TIP=$report,
CMD=_t1_report, END=,\
```

```
NM=t1print_40.gif, NM2=$Print it, TIP=$print,
CMD=_t1_export, END=
```

Notes to this guide definition:

- The original Bruker guides are defined in the file `toolbar.prop` in the directory <tshome>/classes/prop. The corresponding commands are defined in `cmdtab_main.prop` in the same directory.
- The bold lines in the example above are user-modified lines.
- `NM=t1fid_40.gif`: a Bruker defined icon with a size of 40x40 pixels
- `NM=myicon.gif`: a user-defined icon, which must be located in the user properties directory (Caution: not in its subdirectory userdefined)
- `NM=C:/myicons/myicon1.gif`: a user-defined icon located C:/myicons. Using the absolute pathname allows you to store icons in an arbitrary directory.
- `NM=-` : indicates the start of the second icon column
- `NM2=` : the text to appear underneath of the icon. The $ sign is mandatory.
- `CMD=` : the command to be executed when the icon is clicked. This can be a regular TOPSPIN command, a macro or an AU or Python program.
- `TIP=` : the tooltip to be displayed when the cursor is held over the icon. Note that the $ sign is mandatory.

Before you can start a user defined guide, you must edit the file `cmdtab_user.prop` and define the corresponding command in the file, for example:

```
myt1guide=EM=J, MC=N, CL=tutor.TutStarter, ME=startTuto-
rial,AR=MyT1T2Toolbar;My T1 T2 Tutorial=
```

Here:

- `"MyT1T2Toolbar"` is the toolbar identifier as it is used in the file `toolbar_user.prop.`
- `"My T1 T2 Tutorial"` is the title as it appears at the top of the guide.

If your guide is a Bruker modified guide, you can also redefine the original Bruker command, i.e. specify `t1guide` instead of `myt1guide`. Note that the original Bruker guide is then no longer accessible.

If you want to access a user defined guide from the TOPSPIN toolbar, you have to

create a new toolbar button. To do that, right-click in an empty area of the toolbar and define a button in the appearing dialog.

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